ENVIRONMENTAL RESEARCH

RESEARCH AND TECHNOLOGY BRANCH

THE DEVELOPMENT OF A LONG RANGE TRANSPORT MODEL WITH A NESTED FINE RESOLUTION GRID

PHASE II

Ontario
Environment
Environnement

ISBN 0-7778-0558-8

THE DEVELOPMENT OF A LONG RANGE TRANSPORT MODEL WITH A NESTED FINE RESOLUTION GRID

PHASE II

Report prepared for:
Ontario Ministry of the Environment

Report prepared by:
Dr. M. Niewiadomski and L. Shenfeld
The MEP Company

NOVEMBER 1993

Cette publication technique n'est disponible qu'en anglais.

PIBS 2290

ACKNOWLEDGEMENT AND DISCLAIMER

This report was prepared for the Ontario Ministry of Environment and Energy (formerly Ministry of the Environment) as part of a Ministry funded project. The views and ideas expressed in this report are those of the author(s) and do not necessarily reflect the views and policies of the Ministry of Environment and Energy, nor does mention of trade names or commercial products constitute endorsement or recommendation for use. The Ministry, however, encourages the distribution of information and strongly supports technology transfer and diffusion. Note, all references to the Ministry of Environment in the report should read Ministry of Environment and Energy.

Any person who wishes to republish part or all of this report should apply for permission to do so to the Research and Technology Section, Fiscal Planning and Information Management Branch, Ontario Ministry of Environment and Energy, 135 St. Clair Ave. W., Toronto, Ontario, M4V 1P5, Canada.

ABSTRACT

The nested mesoscale modelling system for air pollutants, developed under Phase I of this project, has been changed, to cover an area of approximately 750 x 600 km. The horizontal resolution is 20 km. The new domain includes Southern Ontario and the neighbouring portions of adjacent states.

The model has been applied to simulate a high ozone episode in Southern Ontario. Based on the test runs, the convective boundary layer parameterization in Gesima was improved and optimal values of some input parameters were selected. Analyses were made on the areal distribution of ozone, NO_x, and VOCs and the time series of these species in selected locations: Guelph, Toronto and Oshawa. The results are in fairly good agreement with observations, which is a marked improvement over the results obtained in Phase I with respect to the predicted peak ozone levels.

EXECUTIVE SUMMARY

Two existing numerical models: a German mesoscale meteorological model, Gesima and a long range transport model, Acid Deposition and Oxidant Model (ADOM), have been enhanced, adapted and interfaced under Phase I of this project to form a nested mesoscale modelling system for simulations of the transport, chemical transformations and deposition of atmospheric pollutants. Based on the tests of the model undertaken under Phase II, and described in this report, several significant improvements of the system were made. The domain of simulation has been extended from the domain used in Phase I to cover most of Southern Ontario as well as adjacent areas in the U.S. The horizontal resolution of 20 km used in the model, coupled with the appropriate topography, land use and local emissions data would allow finer local features of ambient pollution and deposition to be simulated.

Two series of tests of the system were undertaken. The test runs of ADOM, showed that the ozone concentration is very sensitive to the inflow boundary concentrations. In order to decrease this sensitivity to boundary inputs, the domain has been extended from that used in Phase I. The second series of test runs focused on selecting the best set of input parameters for Gesima. The results of these tests also led to the replacement of the convective boundary layer parameterization in Gesima and some other modifications of the model.

In order validate the system, a simulation of a high ozone episode in Southern Ontario has been performed. The test run was carried out for a period of 8 days, starting on July 30 1988. The analysis of the results of this run focuses on the areal distribution of ozone, as well as nitric oxides and hydrocarbons, and their diurnal variations in selected locations. The horizontal cross-sections of the ozone, NO_x and VOC concentrations, presented in Figs. 14 to 28 show pronounced mesoscale variability, which cannot be simulated using regional scale air pollution models such as ADOM with horizontal resolution of 127 km as it is used to simulate over eastern North America now. The predicted levels of ozone at three Ontario locations (Guelph, Toronto and Oshawa) were compared to the available observational data. The time series (see Figs. 31 - 34) show a fairly good agreement with observations, especially near ground level. There is a marked improvement over the results obtained in Phase I, with respect to the predicted peak ozone levels.

TABLE OF CONTENTS

1. INTRODUCTION

This report describes the second phase of the development and testing of a nested grid, mesoscale air pollution modelling system, carried out under a contract with the Ontario Ministry of the Environment from July 1991 to June 1992. The test runs of the system are made for a high ozone episode over Southern Ontario in August 1988.

The system is capable of simulating the emission, transport, chemical transformation and deposition of a wide range of air pollutants. Horizontal resolutions of 5 to 20 km can be used. The size of the domain of simulation can vary, depending on resolution and the available computer resources, from about 100 x 100 km to 700 x 700 km or more. The test runs of the system for the Toronto area were carried out with horizontal resolution of 20 km in a domain of 340 x 340 km in Phase I. That domain has been enlarged in this phase to 750 x 600 km without changing the resolution. Thus, the present domain of the system covers most of Southern Ontario.

The resolution and the size of the domain place this system in the mesoscale, i.e. between the urban scale air quality models and the large scale models of long range transport of atmospheric pollutants (LRTAP). The mesoscale modelling capability is necessary to address the urban NO_x/VOC issue with a view to understanding and eventually to controlling the ozone precursor emissions and to quantify the subgrid scale variability of pollutant concentrations simulated by the LRTAP models.

The approach was to adapt, enhance and interface two models: the large scale Acid Deposition and Oxidant Model (ADOM), and a mesoscale meteorological model 'Gesima'. Gesima and the modified mesoscale version of ADOM are then 'nested' in the large scale ADOM domain.

The modelling system developed in this study consists of three main parts: the large scale ADOM, Gesima, and the mesoscale version of ADOM. The programs interfacing these three parts are also an important part of the system. The interactions between the system components are schematically represented in Figure 1. The initial and boundary conditions for the mesoscale ADOM are derived from the large scale ADOM output files made available by the Ontario Ministry of the Environment.

The original large scale version of ADOM uses meteorological fields generated by the Canadian Meteorological Centre (CMC) spectral diagnostic model. These data, having horizontal resolution of 381 km, are interpolated and gridded to the 127 km resolution domain by the ADOM meteorological preprocessor. The

preprocessor also enhances the vertical resolution of the CMC fields by running a one-dimensional boundary layer model between the ground and the 2 km level at each grid point. For details see Scholtz et al., 1986.

The mesoscale ADOM requires three-dimensional fields of meteorological parameters like horizontal and vertical wind velocity, temperature, humidity, turbulent diffusion parameters etc., with horizontal resolution of 20 km. Such fields are, in this project, generated by Gesima. The role of the large scale ADOM is to provide the initial and boundary conditions for the mesoscale simulations. Most of the development work of the system was completed under Phase I of this project. Details are described in the previous report (Niewiadomski and Shenfeld, 1991). The approach of the project, major components of the system and the results of Phase I were also summarized in a paper presented at the Technology Transfer Conference in November 1991 (Niewiadomski, 1991, included in this report as Appendix A) and in a poster presented at the Joint International Conference on Atmospheric Chemistry organized by the Canadian Institute for Research in Atmospheric Chemistry and the Ontario Section of AWMA in January 1992.

Phase II of this project focused on testing, fine tuning and improving the system. Two types of tests were made, studying the response of ADOM to changes in the boundary conditions and point source emissions within the domain and the response of Gesima to changing the "nudging" coefficient. The optimal choice of other input parameters of the model was also determined. These test runs and their results are described in Sections 2 and 3. The tests led to a modification of the boundary layer module of Gesima which is described in Section 4. Section 5 presents some results of the first "production runs" of the system performed for the Ministry of the Environment in May and June 1992 as a part of the emission trading scenarios project. The adopted set of input parameters is provided in Appendix B. Appendix C describes in detail the modifications of the Gesima subroutines undertaken during Phase II. Short descriptions of all Gesima subroutines are included in Appendix D.

A significant amount of time was also devoted to the technical problems resulting from changes in hardware and software due to the transfer of the system in April 1992 from the Cray computer of the Ontario Centre for Large Scale Computation to the Cray and SX-3 computers at the Environment Canada Centre Informatique de Dorval. The system is now fully operational at C.I.D. Its Gesima part operates on the new SX-3 supercomputer, while ADOM, containing some Cray-specific library subroutines, is currently run on the C.I.D Cray.

2. TORONTO AREA TESTS

At the beginning of this project several test runs of the system were performed using the same domain of simulations as in Phase I. These tests focused on the relative importance of boundary conditions and local point source emissions on ozone concentrations simulated by the mesoscale version of ADOM.

The tests period covered August 1 to August 4, 1988. The mesoscale ADOM was run using the meteorological fields generated by Gesima during Phase I. For details on Gesima runs and the map of the domain, see the Phase I report (Niewiadomski and Shenfeld, 1991). The output files of large scale ADOM, which provided the initial and boundary conditions for these tests, were produced by an improved version of ADOM that included a mass conservation module.

The mesoscale ADOM was run with artificially increased and decreased boundary concentrations of ozone and NO_x. Tests were carried out including and excluding two large NO_x sources in the area: Nanticoke and Lakeview generating stations. Selected results of these tests are presented in Figures 2 - 7.

The comparison of Figures 2 and 3 shows that a 100% increase in boundary ozone concentrations resulted at 8:00 p.m. EDT in an increase of ozone by 50 to 80% throughout the domain, without radically changing the areal distribution pattern. Additional increase of the NO_x boundary values (see Figure 4) does not introduce significant changes. For the Toronto location (see Figure 6), the afternoon O_3 maxima increased by about 80% and the effect of an additional increase of boundary NO_x values was negligible. Reducing the boundary concentrations by 90% resulted in the reduction of maximum O_3 by 60% to about 25 ppb. Thus, the emissions from inside the domain contributed only to 40% of the simulated base case maximum Toronto ozone concentration. The contributions of single sources is much lower, as can be seen from Figure 7 which shows O_3 time series for the case with Lakeview emissions excluded.

The dependence on boundary conditions, which are derived from the large scale ADOM results and thus do not have sufficient resolution, brings into question the validity of using such a small domain for mesoscale simulations. It was decided that instead of running the model in smaller domains separately e.g. for the Toronto and Windsor areas, the domain should be large enough not only to cover most areas of interest but also to move the boundaries of the domain far from those areas. As can be seen from Figure 8, the new larger domain fulfils the latter condition much better for Toronto than for Windsor.

3. SOUTHERN ONTARIO TESTS

3.1 Domain of Simulations and the Set-Up of the Experiment

The new large domain of simulation is shown in Figure 8. It covers 6 x 5 grid cells of the large scale ADOM domain (with x and y coordinates 13 to 18 and 15 to 19, respectively). To obtain the horizontal resolution of about 20 km this area has been divided into 37 x 29 cells. Note that due to the peculiarities of the graphic software used, the grid shown in Figure 8 and in the subsequent figures does not contain zero numbered lines, so the grid lines in the figures correspond to the centres of the grid cells rather then to their borders.

As in Phase I, the basic vertical structure of the large scale ADOM, with 12 variable depth layers, has been retained for the mesoscale version of the model. The tops of the ADOM layers are located at 56.2, 135.8, 250.7, 416.3, 655.3, 1000.0, 1497.2, 2214.5, 3249.2, 4741.6, 6894.5, and 10000.0 m above the ground level. As in Phase I, Gesima uses 16 vertical layers, with each of the 4 top layers of ADOM corresponding to two Gesima's layers. Thus the tops of Gesima layers lie at 56.2, 135.8, 250.7, 416.3, 655.3, 1000.0, 1497.2, 2214.5, 2731.8, 3249.2, 3995.4, 4741.6, 5818.1, 6894.5, 8447.3, and 10000.0 m. The Gesima/ADOM interface program averages the data from top layers of Gesima and assigns them to the appropriate layers of ADOM. Note that the heights of the layer tops given above are relative to the average topographic height of the grid cell.

Similar to Phase I, the well documented high ozone episode in August 1988 has been selected for simulations, but the period has been extended from 4 to 8 days, starting on July 30 1988. The large scale ADOM output files were obtained by a new simulation on a reduced (33 x 21) horizontal domain. Twelve southern rows of the original grid were removed and higher concentrations ozone were imposed on the new southern boundary, where ozone levels had been underpredicted by the ADOM model in previous runs. These higher values were derived from hourly surface observations interpolated throughout the boundary layer to match predictions of ADOM run on the full domain (33 x 33 grid cells. The boundary conditions for other species were derived from a former simulation on a full grid. The southern boundary of the mesoscale domain is located 254 km north of the south boundary of the 33 x 21 grid domain of the large scale ADOM.

Some input data files of Gesima and mesoscale ADOM have been prepared in a different way than in Phase I. The Ministry of the Environment made available the topography and land use data files for the mesoscale domain, so these files were used directly as

input to Gesima and to prepare the geophysical input file of the mesoscale ADOM. This made redundant some interpolation algorithms in Gesima. Furthermore, since the land use classes used in Phase I in Gesima differed from those of ADOM, the Gesima classes have been redefined so that the same input data sets can be used for both models. For details see Section C.2 of the Appendix C.

3.2 Results

The tests described in this section focus on the sensitivity of the Gesima results to the value of the nudging coefficient. For the discussion of the nudging terms see Section 2.4 of the Phase I report. Analysis of the results of these runs led not only to the selection of proper nudging coefficients, but also to several improvements of the system and to better selection of other input data. The most important improvement was the modification of the boundary layer module of Gesima, described in detail in Section 4. Others included minor modifications of the surface layer module, and changes to the radiation scheme (for details see Appendix C). The values of the input parameters selected as a result of these tests are listed in Appendix B.

Tests also showed that the boundary conditions scheme for the cloud variables in Gesima (see Section A1.5 of the Phase I report) introduced some errors to the results. The horizontal resolution of 20 km was also too coarse to properly simulate the convective clouds. Since the clouds do not play an important role in the episode studied, it was decided to exclude the whole cloud module, until its boundary condition scheme can be fully tested and improved. The effects of clouds on incoming solar and atmospheric radiation in the surface layer are parameterized according to the interpolated large scale cloudiness data. For details see Appendix C.

Several test runs with different nudging coefficients were performed. As expected, increasing the value of the nudging coefficient led to greater suppression of mesoscale effects, and consequently greater uniformity over the domain while decreasing the nudging coefficient resulted in the mesoscale fields becoming inconsistent with the large scale meteorological situation. Based on these tests, a vertically uniform nudging coefficient of 0.0001 per second was chosen for all variables. The surface wind fields simulated with this coefficient for August 2, 1988 are compared to the winds i.e. interpolated from the large scale data in Figures 9 - 13. As can be seen the mesoscale winds, while retaining some local features follow the main large scale flow.

Even so, it takes several hours for any significant change in the large scale situation to be reflected in the simulated mesoscale fields.

4. NEW CONVECTIVE BOUNDARY LAYER SCHEME FOR GESIMA

The original Gesima determined the turbulent diffusivity coefficients for momentum and heat at the height z according to the following formulae:

$$K_{zm} = (m / \phi_m)^2 \; S \quad if \quad \partial\theta/\partial z > 0 \tag{1}$$

$$K_{zm} = m^2 \; (S^2 - 15B)^{1/2} \quad if \quad \partial\theta/\partial z < 0 \tag{2}$$

$$K_{zH} = K_{zm} D \tag{3}$$

where ϕ_m is a stability function computed according to Bussinger et al. (1971), $m = kz / (1 + kz/\lambda_m))$ is the mixing length computed according to Blackadar (1962) and Mellor and Yamada (1974). $S = ((\partial u/\partial z)^2 + (\partial v/\partial z)^2)^{1/2}$ and $B = (g/\Theta)(\partial\theta/\partial z)$ denote the wind shear and buoyancy parameter, respectively, while $k = 0.4$ is the von Karman's constant. D is a coefficient based on the Richardson's number and λ_m is a function of the Coriolis parameter and the mean geostrophic wind.

The model tests showed that for resolution of 20 km the above formulation, which was originally designed to be run with horizontal grid sizes of 2 to 5 km, led to underestimated diffusivities in cases of convective conditions. The mixed layer extended up only several hundred meters or less, even on a sunny summer afternoon when the mixing height could be up to 2000 meters.

Equation (2) for K_m during convective conditions was changed based on the approach of Hass (1991) to the following:

$$K_m = k \; w_* \; z \; (1 - z/Z_i) \tag{4}$$

where Z_i is the mixed layer height.

The convective velocity scale (w_*) is computed from the formula:

$$w_* = (g \; H \; Z_i \; / (T \; c_p \rho))^{1/3} \tag{5}$$

where ρ and c_p are density and specific heat of air and T denotes the average temperature in the mixed layer. The surface heat flux

(H) is computed in the surface layer module of Gesima. Since the mixed layer height (Z_i) is not directly available in Gesima, its value is interpolated from the low resolution input data of the large scale ADOM.

The criterion for applying the convective formulation is now based on the sign of H so that equation (4) is used for $z < Z_i$ only if the surface heat flux is directed upwards. In all other cases equation (1) applies as before. The diffusivity coefficient for heat is computed according to equation (3) as in the original Gesima.

The difference between the new and original formulations is illustrated below in Table 1, showing vertical profiles of turbulent diffusion coefficient at 4.00 p.m. EDT on August 1, 1988 for a grid cell NE of Toronto. Z_i for that case was equal to 1130 m, and w_* to 0.50 m/s.

Table 1. Sample diffusivity profiles

		original formulation		modified formulation	
level	z	K_m	K_H	K_m	K_H
1	56	0.139E+01	0.221E+01	0.328E+02	0.521E+02
2	136	0.964E+00	0.122E+01	0.405E+02	0.511E+02
3	251	0.325E-02	0.328E-02	0.489E+02	0.495E+02
4	416	0.365E-02	0.369E-02	0.553E+02	0.559E+02
5	655	0.404E-02	0.408E-02	0.527E+02	0.533E+02
6	1000	0.630E-02	0.637E-02	0.243E+02	0.246E+02
7	1497	0.617E-02	0.624E-02	0.617E-02	0.624E-02
8	2214	0.500E-01	0.506E-01	0.500E-02	0.506E-02
9	2731	0.757E-02	0.766E-02	0.757E-02	0.766E-02
10	3249	0.366E-02	0.369E-02	0.366E-02	0.369E-02
11	3995	0.283E-02	0.286E-02	0.283E-02	0.286E-02
12	4742	0.115E-02	0.116E-02	0.115E-02	0.116E-02
13	5818	0.267E-02	0.269E-02	0.267E-02	0.269E-02
14	6894	0.141E-02	0.142E-02	0.141E-02	0.142E-02
15	8447	0.872E-03	0.881E-03	0.872E-03	0.881E-03
16	10000	0.872E-03	0.881E-03	0.872E-03	0.881E-03

5. EMISSION TRADING RUNS

5.1 Introduction

After the completion of the Gesima tests described in Section 3, several runs of the system were performed as a part of the emission trading project of the Ontario Ministry of the Environment. The meteorological fields were produced by Gesima for the period July 30 to August 6, 1988 in the domain described in Section 3.1 and shown in Figure 8. Mesoscale ADOM was run for the same period, using emission data provided by O.M.E., representing 4 different emission scenarios.

The results for various scenarios will be described in a separate report. The ozone distribution for the base case, which has the input emissions most closely corresponding to the actual emissions in 1988, is discussed below.

5.2 Areal Distribution of pollutants

Contours of the level 1 simulated ozone concentration at 4:00 p.m. EDT (i.e. close to the daily ozone peaks) on each day of the period are presented in Figs. 14 to 21. Figure 22 shows the ozone concentration at 4 a.m. on August 2 1988 and Figs. 23 - 28 the concentrations of NO, NO_2 and VOCs at 4 a.m. and 4 p.m. of that day. The VOC levels in Figs. 27 - 28 (and Figs. 29 - 30 as well) represent combined concentrations of 11 ADOM species, computed according to a formula provided by O.M.E.

As expected, the areas of highest ozone concentration are located downwind of major urban areas, Detroit/Windsor, Cleveland and Toronto. At night these areas have the lowest O_3 concentrations due to scavenging by NO_x. The higher ozone concentrations over the Great Lakes are caused by the lower diffusivity and dry deposition over water than over land.

5.3 Diurnal Variations and Comparison with Observations

The time evolution of concentrations of ozone, NO, NO_2 and VOCs modelled at level 1 of the model on August 2, 1988 are shown for the Toronto and Guelph cells in Figs. 29 and 30, respectively. At both locations NO_x and VOCs peak at the same time: 9 a.m. EDT. The afternoon peak of ozone occurs in Toronto at 4:00 p.m, one hour later than in Guelph. The concentrations of NO and VOCs are an order of magnitude greater in Toronto than in Guelph. Toronto has twice the Guelph NO_2 concentration. The ozone peak in Toronto is, however, only slightly higher than in Guelph,

indicating the importance of the ratio of VOC to NO_x rather than their individual magnitudes in the development of ozone.

The plots of the time evolution of the modelled ozone concentration in selected locations are given in Figs. 31 to 34. The results for the model layers 1 and 4 of the Toronto cell (Figs. 31, 32) are given for the whole period of simulation, while those for the lowest level of the grid cells containing Guelph (Fig. 33) and Oshawa (Fig. 34) cover only the middle part of the period (August 1 to 4). Note that similar plots were presented for the same locations in the report of Phase I (Niewiadomski and Shenfeld, 1991).

In order to validate the ozone levels as computed by the ADOM/Gesima approach, the simulated concentrations are compared to the levels measured from August 1 to 4, 1988, in one hour intervals, at the Air Quality Index (AQI) stations at the heart of downtown Toronto (Fig. 31) and at the top of CN Tower (Fig. 32). Similar measurements from the AQI stations in Guelph and Oshawa are included in Figs. 33 and 34.

It should be noted that while the measurements were taken at specified points, the modelled concentrations represent averages from a mesoscale ADOM cell of the size 20 x 20 km and a depth of 56 m for level 1 and a depth of 165 m for level 4. Even so, the modelled and observed ozone concentrations are in generally good agreement. Although the model does not predict the highest measured concentrations (e.g. 112 ppb observed in Toronto on August 2, 1988 at 14:00 EDT versus 75 ppb modelled), such discrepancies result, at least partly, from the incompatibility between point measurements and the model's volume averaged concentrations.

The times of maximum and minimum modelled concentrations coincide with those observed at the surface in all three locations (except for the secondary peaks in observed concentrations at the early morning of August 4, 1988, in Toronto and Oshawa, which are not reflected in the model results and a secondary peak in model results at the early morning of August 2 in Guelph which is not reflected in measurements). In general, the modelled minima tend to have lower concentrations and last longer than the observed ones.

The upper level data, both modelled and observed, have much less regular diurnal variability (see Fig. 32). The CN Tower is close to the tall buildings in downtown Toronto, so the turbulence structure is rather complicated. This may explain the large fluctuation in the observed ozone concentrations. At the higher altitude there is no removal of ozone due to deposition and less scavenging due to the automobile emissions of nitric oxide than at ground level. The modelled concentrations generally

agree with the observed levels. The largest discrepancy occurs at 6:00 EDT on August 4, 1988. Neither the peak in the model results at that time, nor the minimum in observed levels can be explained by meteorological or other input parameters.

A remarkable improvement, especially for the lowest layer, can be seen when comparing Figs. 31 - 34 to corresponding results of Phase I (Figs. 113 - 116 of Niewiadomski and Shenfeld, 1991 and Fig. 2 of Appendix A of this report). The increase in the modelled ozone concentrations during the afternoon peaks (which however still do not, in several cases, reach the observed values) can be attributed to improvements in the input emission files, southern boundary conditions of the large scale ADOM and the improvements of the diffusivity parameterization in Gesima. Improvement in the timing of the ozone peaks, especially in Guelph, results probably from increasing the model domain (which moved the western boundary of the domain much further from that station) and the mass conservation correction in the large scale ADOM, introduced after the completion of Phase I.

6. SUMMARY AND CONCLUSIONS

A mesoscale modelling system for simulating the transport, chemical transformations and deposition of atmospheric pollutants, designed, developed and preliminarily tested under Phase I of this project, has been extended to cover most of Southern Ontario. Knowledge gained from the test runs resulted in significant improvements of all components of the system, especially the turbulent diffusion parameterization in Gesima, and better selection of adjustable input parameters.

In May and June 1992 the first "production runs" of the system have been performed, as a part of the Ontario Ministry of the Environment emission trading project.

Preliminary analyses of the simulation of the August 1988 high ozone episode over Southern Ontario showed reasonably good agreement of the model results with observations and a marked improvement over the Phase I results.

The system is capable of simulating the distribution of various air pollutants with the spatial resolution of 20 km or less. It can detect local effect of this scale, which is impossible to simulate with large scale models like the original version of ADOM.

More comprehensive analysis of the results of several case studies, and further improvements of the system, including decreasing the grid size to 5 x 5 km, are planned for Phase III of this project to be carried out from July 1992 to June 1993.

7. ACKNOWLEDGEMENTS

We would like to thank the following Ministry of the Environment, Air Resources Branch personnel; Drs. P.K. Misra, C. Fung, R. Bloxam and Mr. S. Wong for their assistance in this study.

8. REFERENCES

Blackadar, A.K. (1962) The vertical distribution of wind and turbulent exchange in a neutral atmosphere. J. Geophys. Res., 67, 3095 - 3102.

Businger, J.A., J.C. Wyngaard, Y. Izumi and E.F. Bradley (1971) Flux-profile relationships in the atmospheric surface Layer. J. Atmos. Sci., 28, 181 -189.

Hass H. (1991) Description of the EURAD chemistry-transport model version 2 (ETM2). Mitteilungen aus dem Institut fur Geophysik und Meteorologie der Universitat zu Koln. Koln, 1991.

Mellor, G.L. and T. Yamada (1974) A hierarchy of turbulence closure models for planetary boundary layers. J.Atmos. Sci.,31, 1791-1806.

Niewiadomski M. and L. Shenfeld (1991) The development of a long range transport model with a nested fine resolution grid. The MEP Company report for the Ontario Ministry of the Environment. June 1991.

Niewiadomski M. (1991) The development of a long range transport model with a nested fine resolution grid. Proc. Technology Transfer Conf. Toronto, November 25 - 26, 1991., pp 42-49.

Scholtz M.T., B. Weisman, L. Mahrt and A.D. Christie (1986) Generation of meteorological data fields for the ADOM Eulerian regional model. Fifth Joint AMS/APCA Conference on Applications of Air Pollution Meteorology, Chapell Hill, NC, pp. 145 - 150.

LIST OF FIGURES

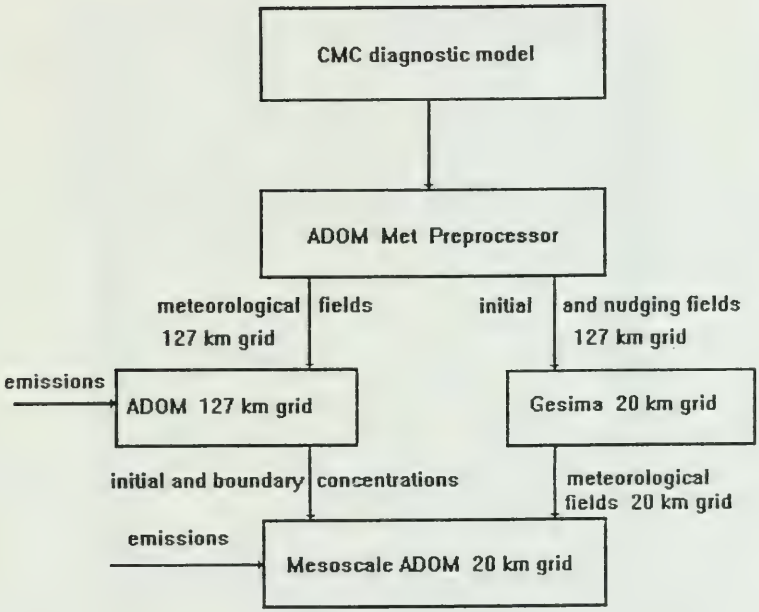


Figure 1. Components and scheme of operation of the nested mesoscale modelling system.

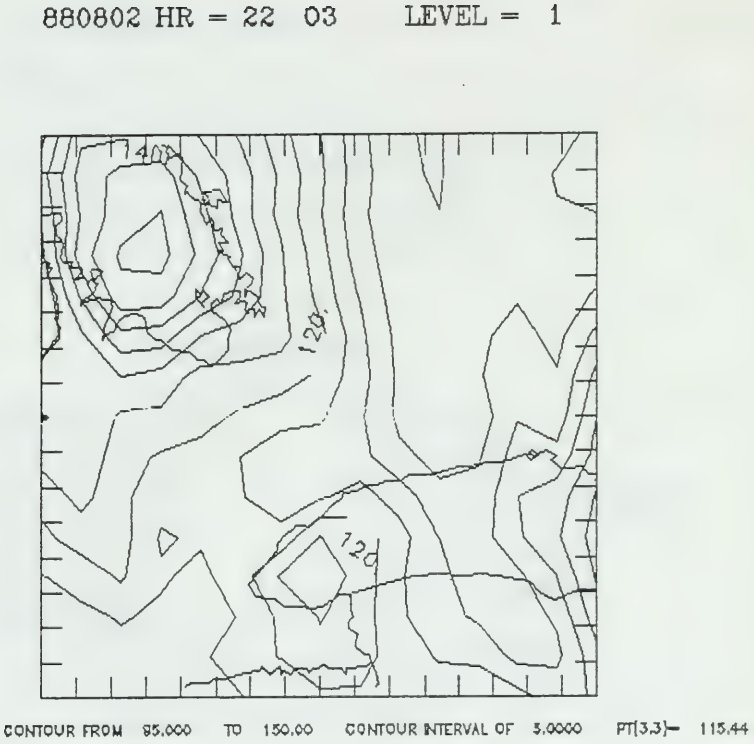
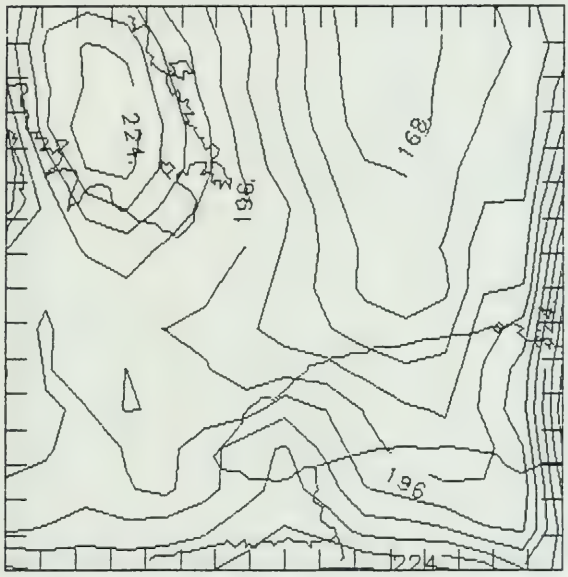


Figure 2: Simulated ozone concentrations (in ug per cubic meter) at 8:00 p.m. EDT on August 2, 1988, base case.

880802 HR = 22 03 LEVEL = 1



CONTOUR FROM 161.00 TO 238.00 CONTOUR INTERVAL OF 7.0000 PT(3,3)= 207.66

Figure 3: Simulated ozone concentrations (in ug per cubic meter) at 8:00 p.m. EDT on August 2, 1988, boundary concentrations of ozone increased by 100%.

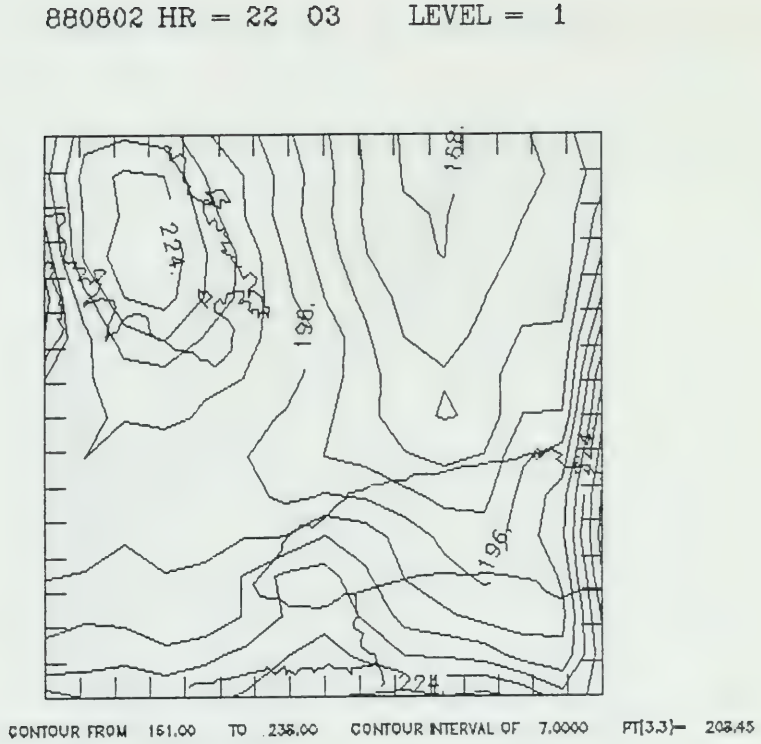


Figure 4: Simulated ozone concentrations (in ug per cubic meter) at 8:00 p.m. EDT on August 2, 1988, boundary concentrations of ozone and NOx increased by 100%.

880802 HR = 22 03 LEVEL = 1

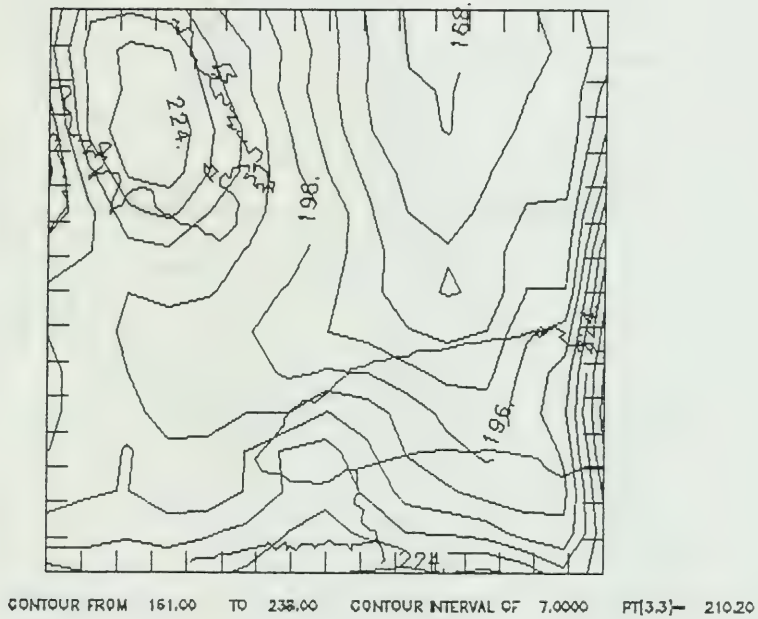


Figure 5: Simulated ozone concentrations (in ug per cubic meter) at 8:00 p.m. EDT on August 2, 1988, boundary concentrations of ozone and NOx increased by 100%, Lakeview and Nanticoke sources removed.

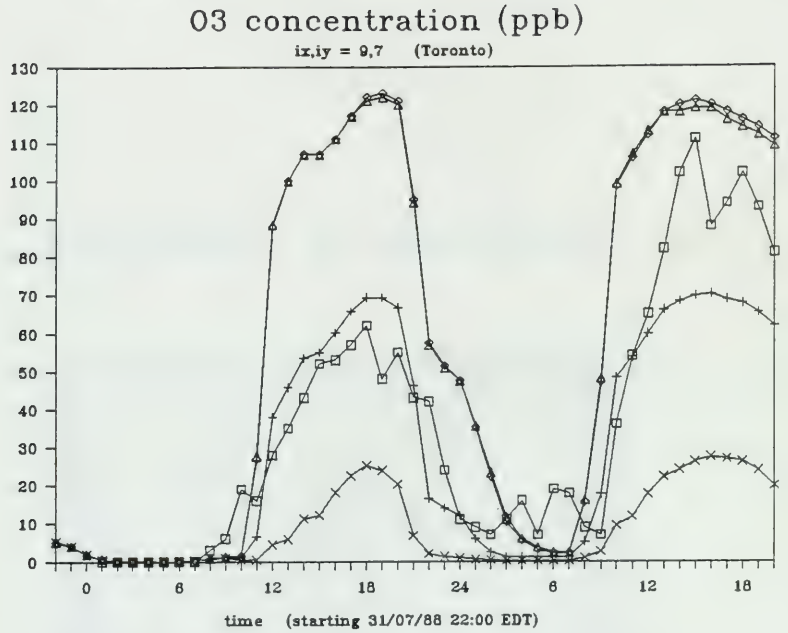


Figure 6. □ observed, + base case, △ b.c. x 2 (O_3)
◇ b.c. x 2 (O_3, NO_x), × b.c. x 0.1 (O_3, NO_x)

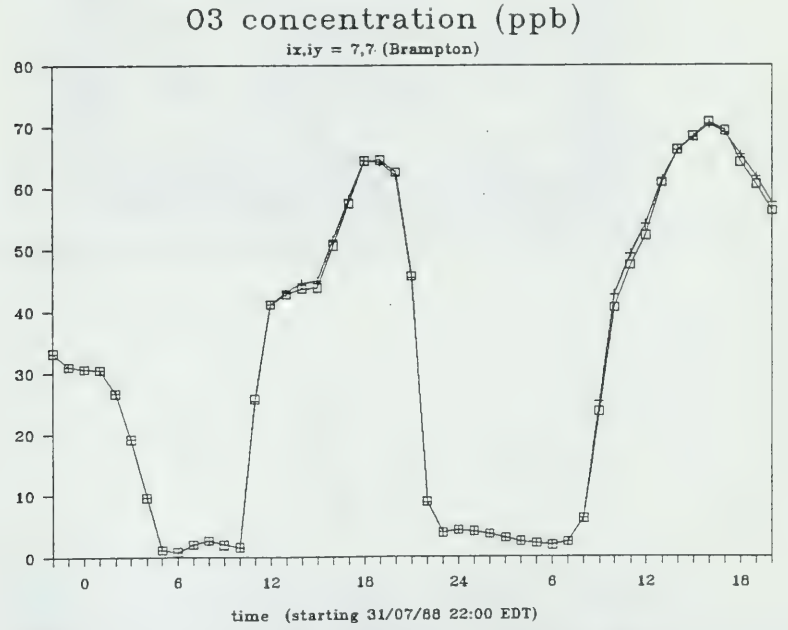


Figure 7. □ base case + Lakeview, Nanticoke removed.

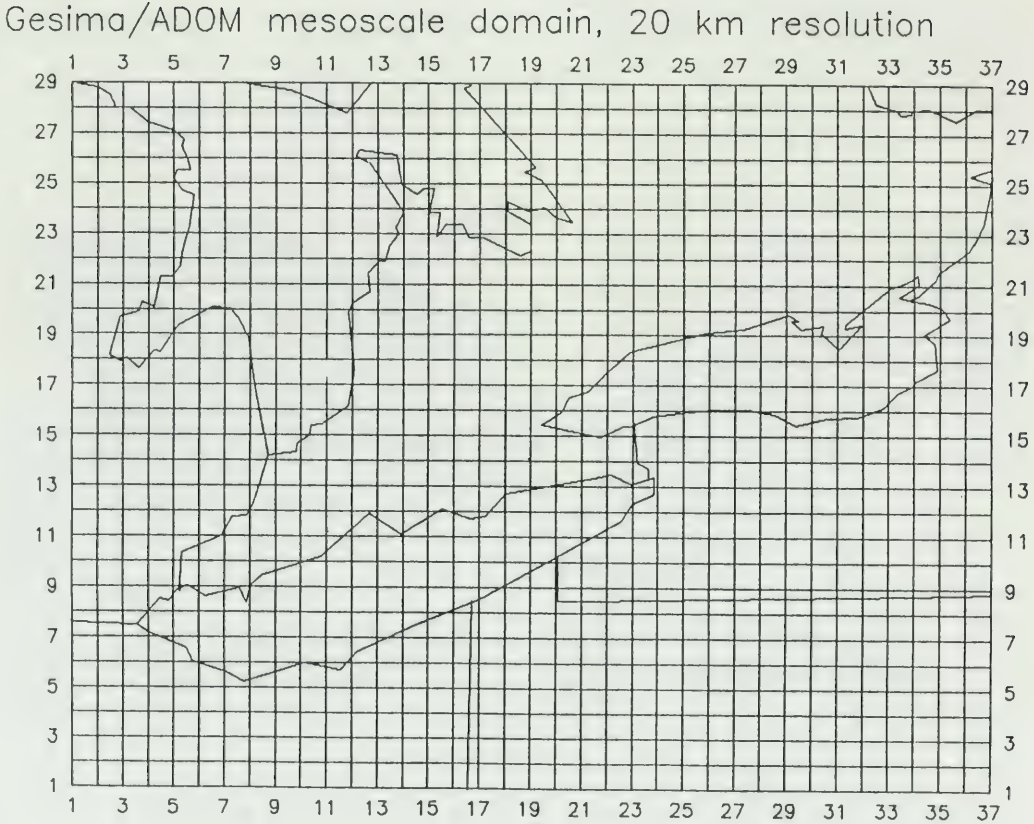
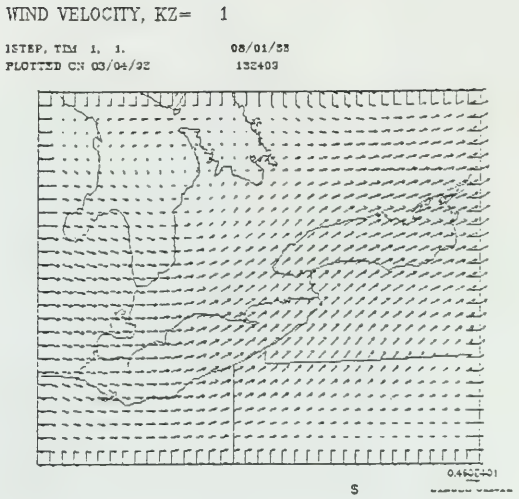

Gesima/ADOM mesoscale domain, 20 km resolution
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1

Figure 8.



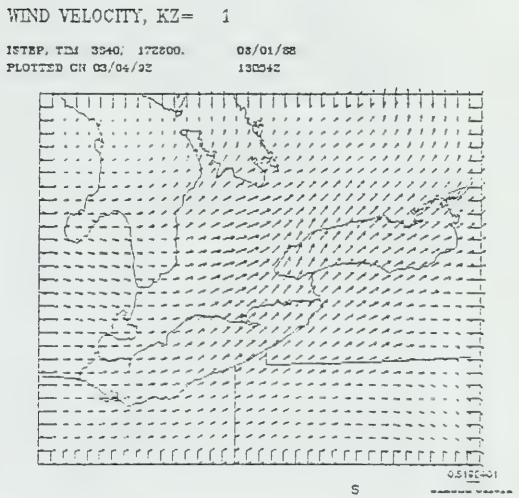


Figure 9: Surface wind fields at 00:00 GMT on August 2, 1988;
top: interpolated from large scale data,
botton: simulated by Gesima

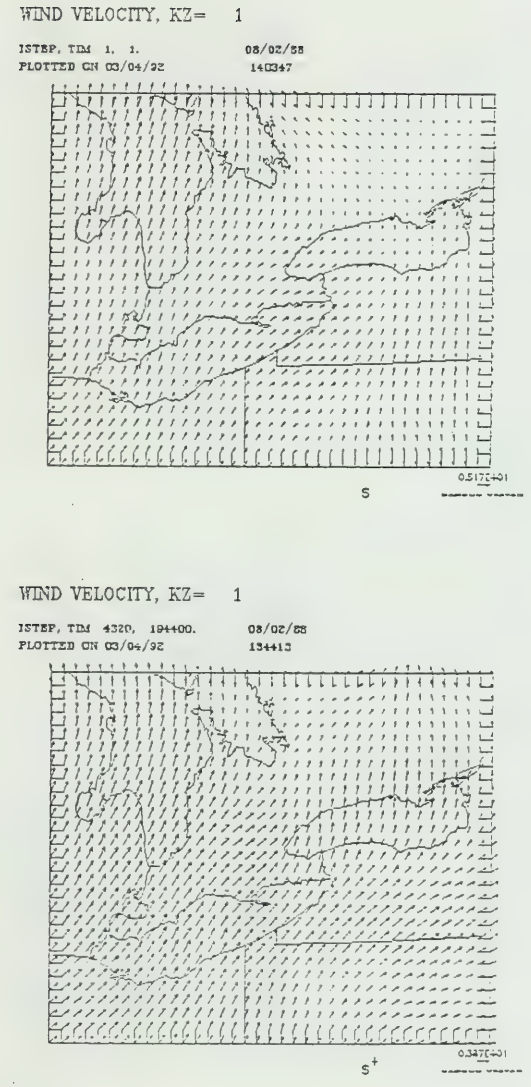
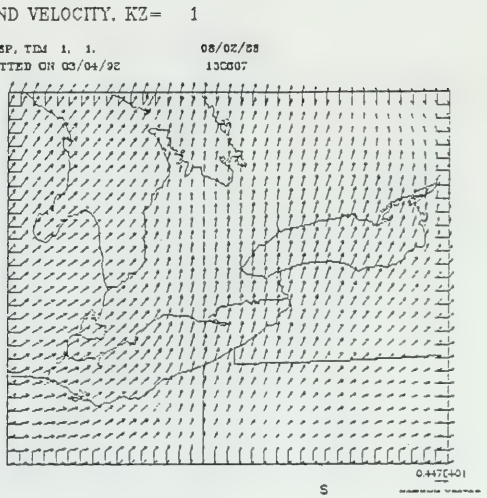


Figure 10: Surface wind fields at 06:00 GMT on August 2, 1988;
top: interpolated from large scale data,
bottom: simulated by Gesima



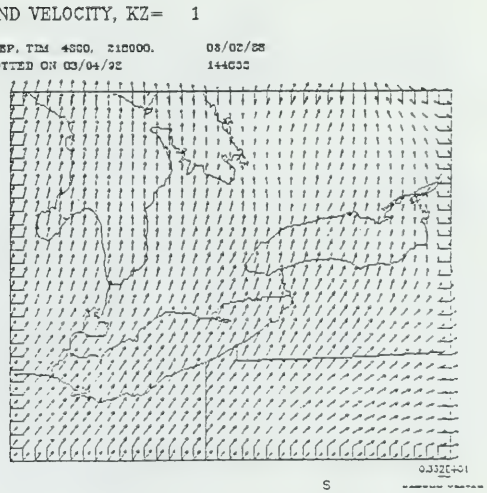
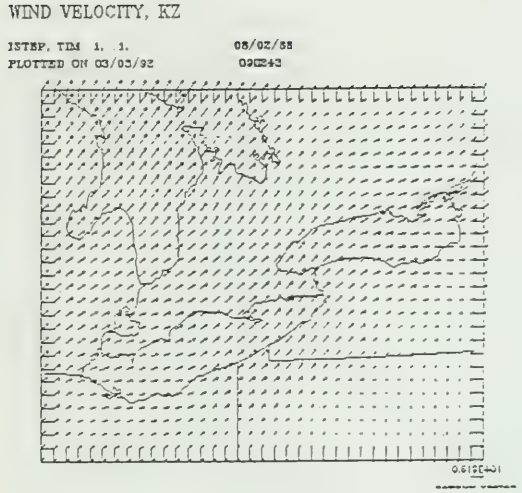


Figure 11: Surface wind fields at 12:00 GMT on August 2, 1988;
top: interpolated from large scale data,
bottom: simulated by Gesima



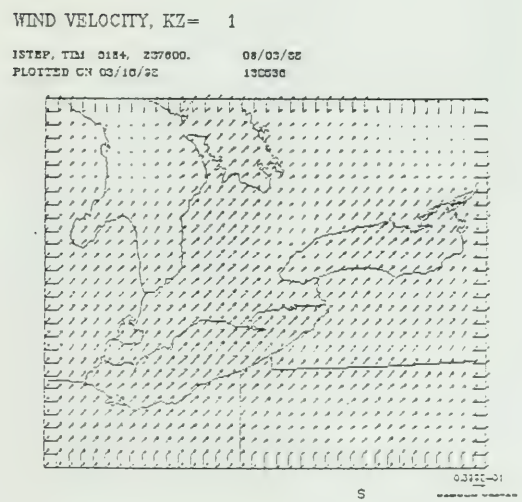
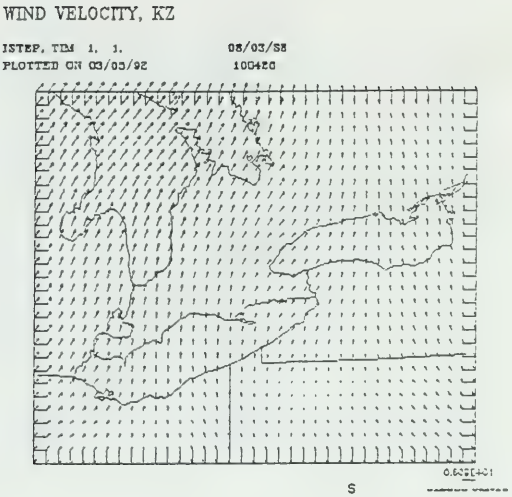


Figure 12: Surface wind fields at 18:00 GMT on August 2, 1988;
top: interpolated from large scale data,
bottom: simulated by Gesima



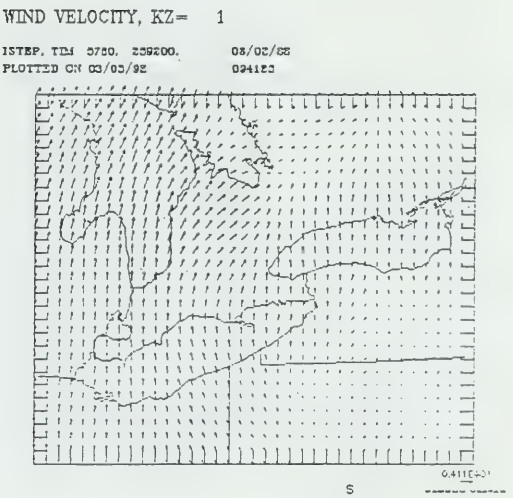


Figure 13: Surface wind fields at 24:00 GMT on August 2, 1988;
top: interpolated from large scale data,
bottom: simulated by Gesima

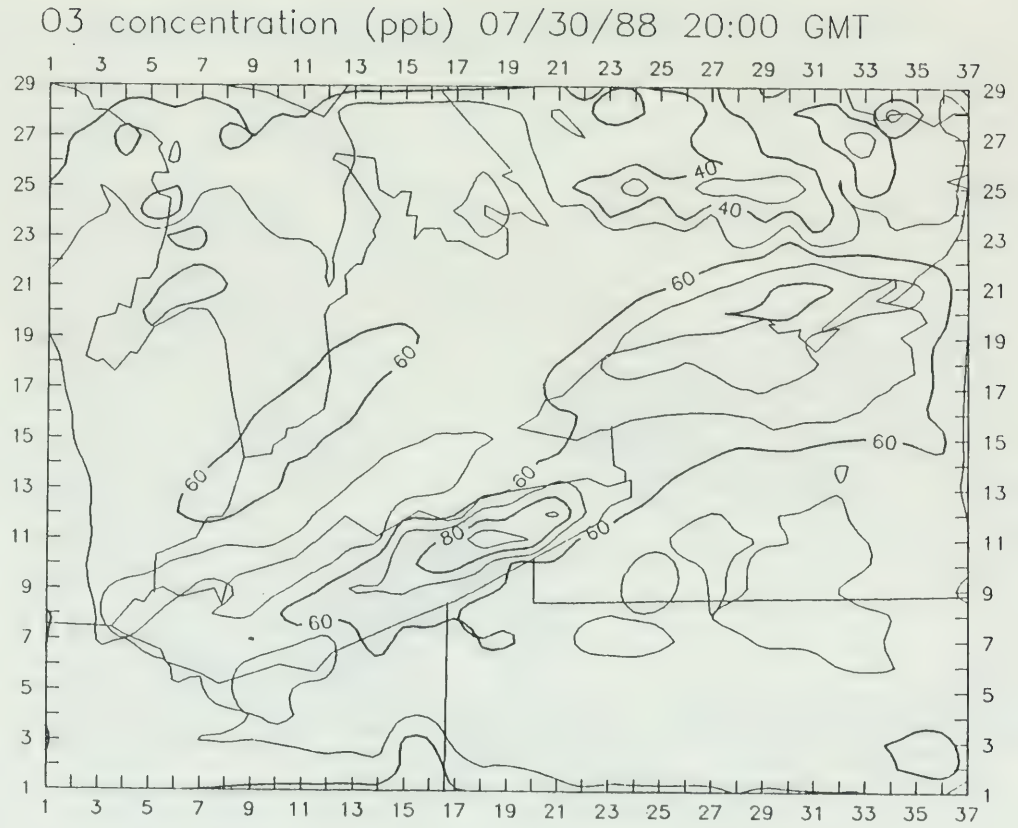

O3 concentration (ppb) 07/30/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
40
40
60
60
60
60
60
60
80
60

Figure 14.

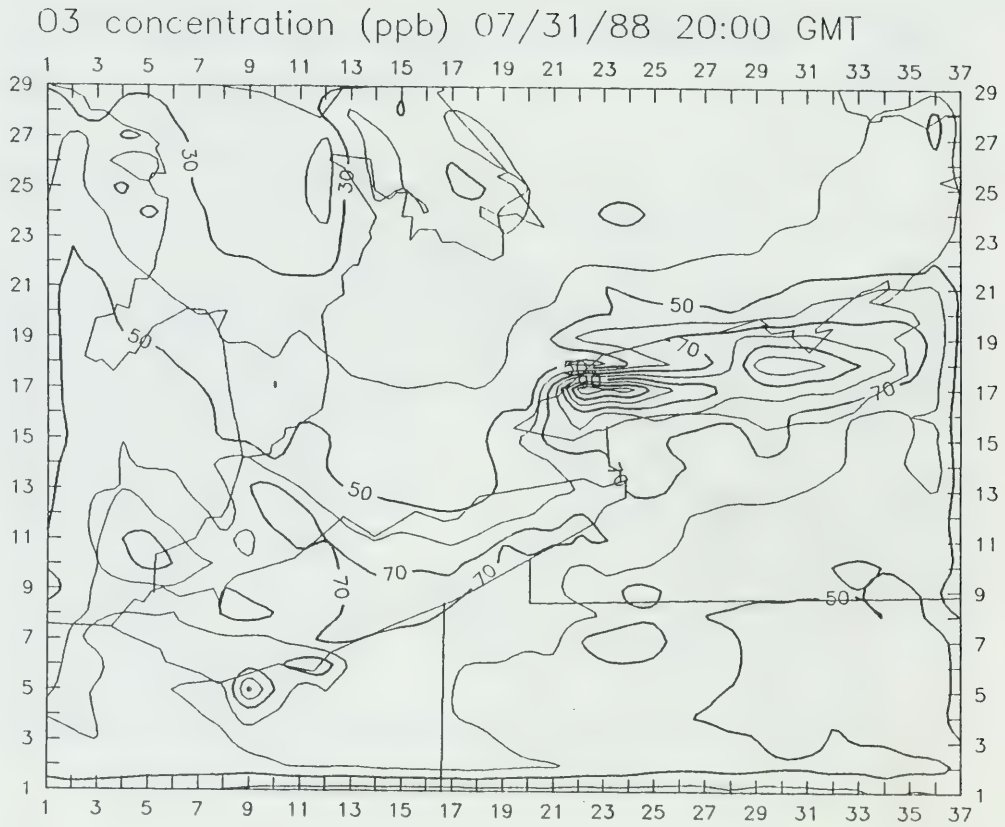

O3 concentration (ppb) 07/31/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
30
30
50
50
70
70
70
70
50
50

Figure 15.

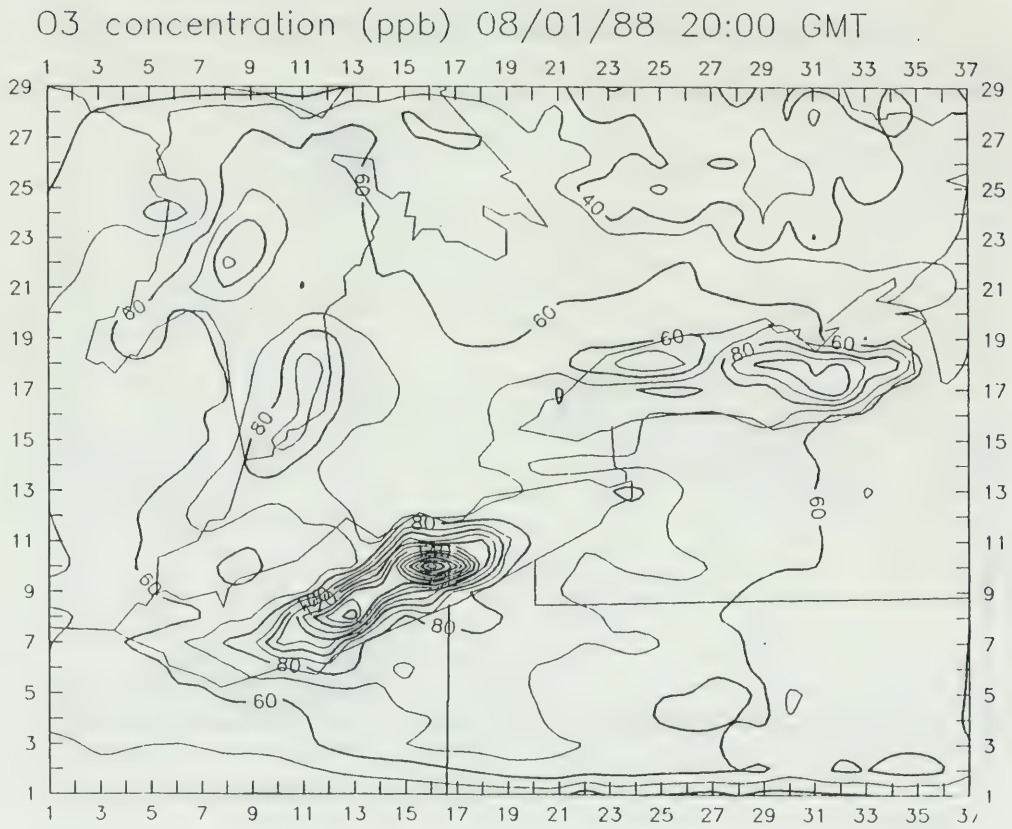

O3 concentration (ppb) 08/01/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
40
60
80
100
120
140

Figure 16.

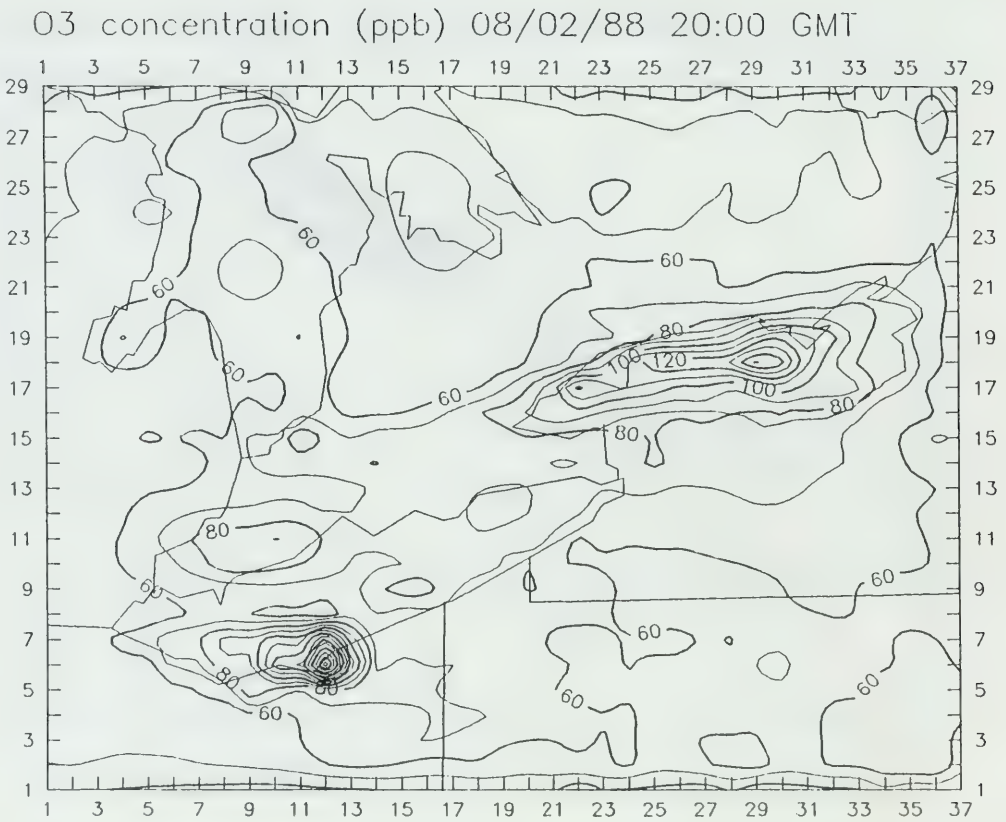

O3 concentration (ppb) 08/02/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
60
80
100
120

Figure 17.

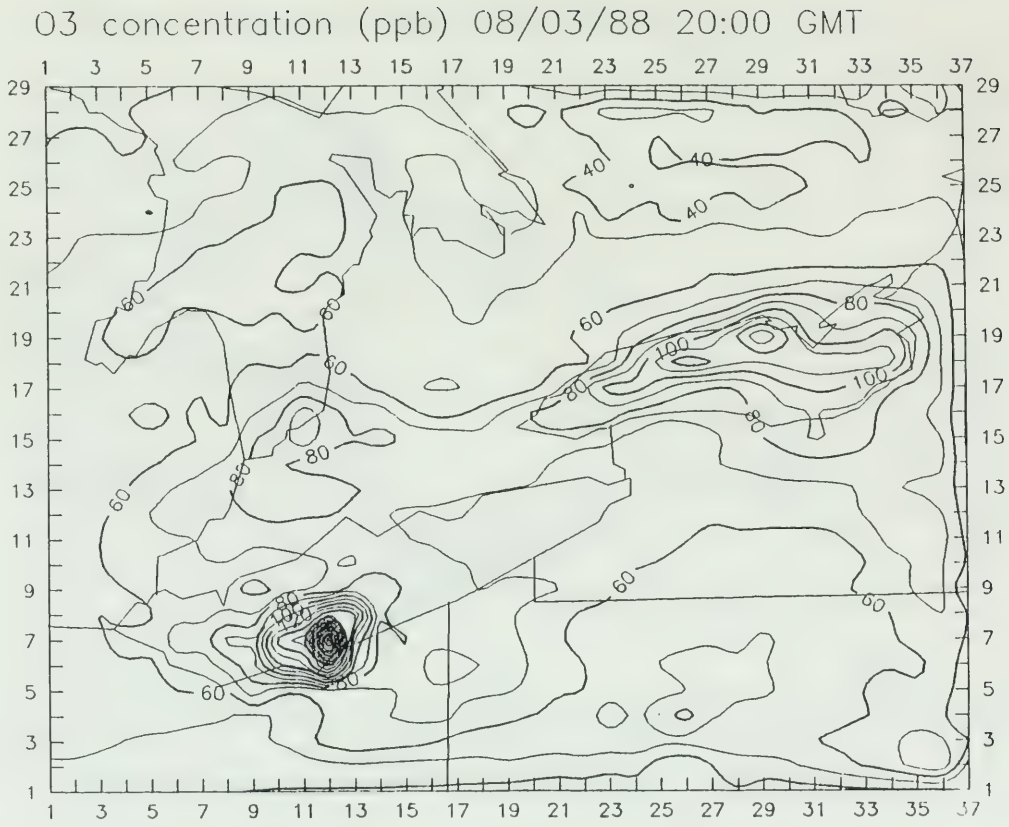

O3 concentration (ppb) 08/03/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
40
60
80
100
120
140

Figure 18.

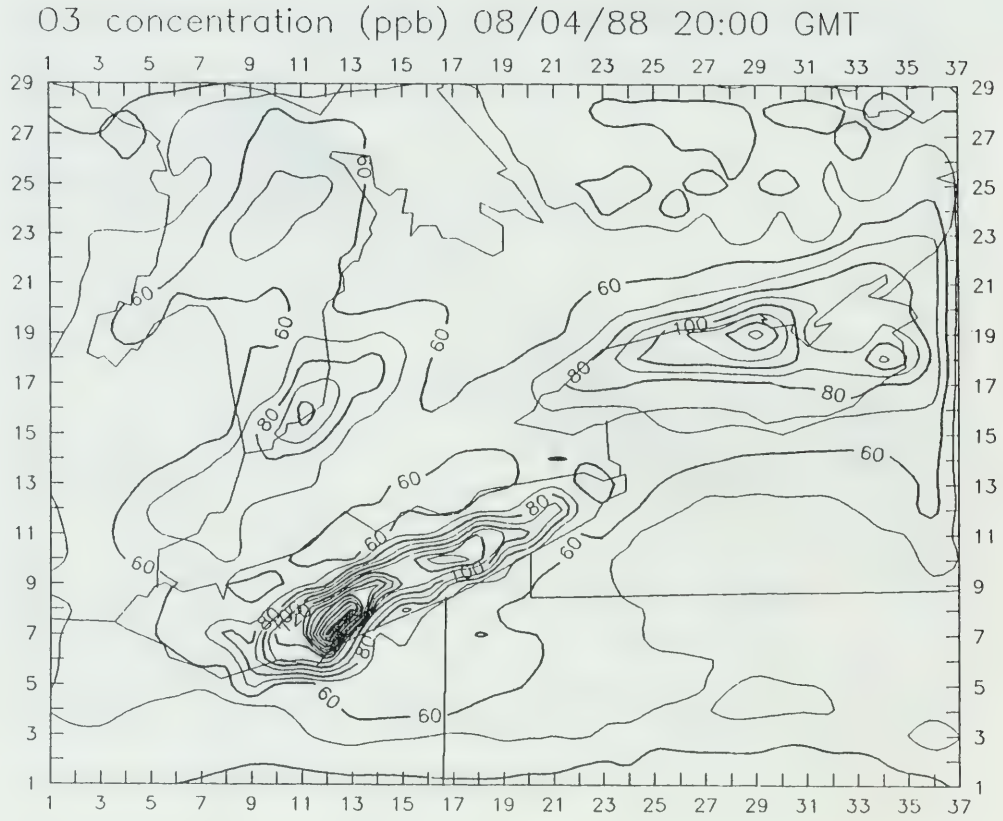

O3 concentration (ppb) 08/04/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
60
80
100

Figure 19.

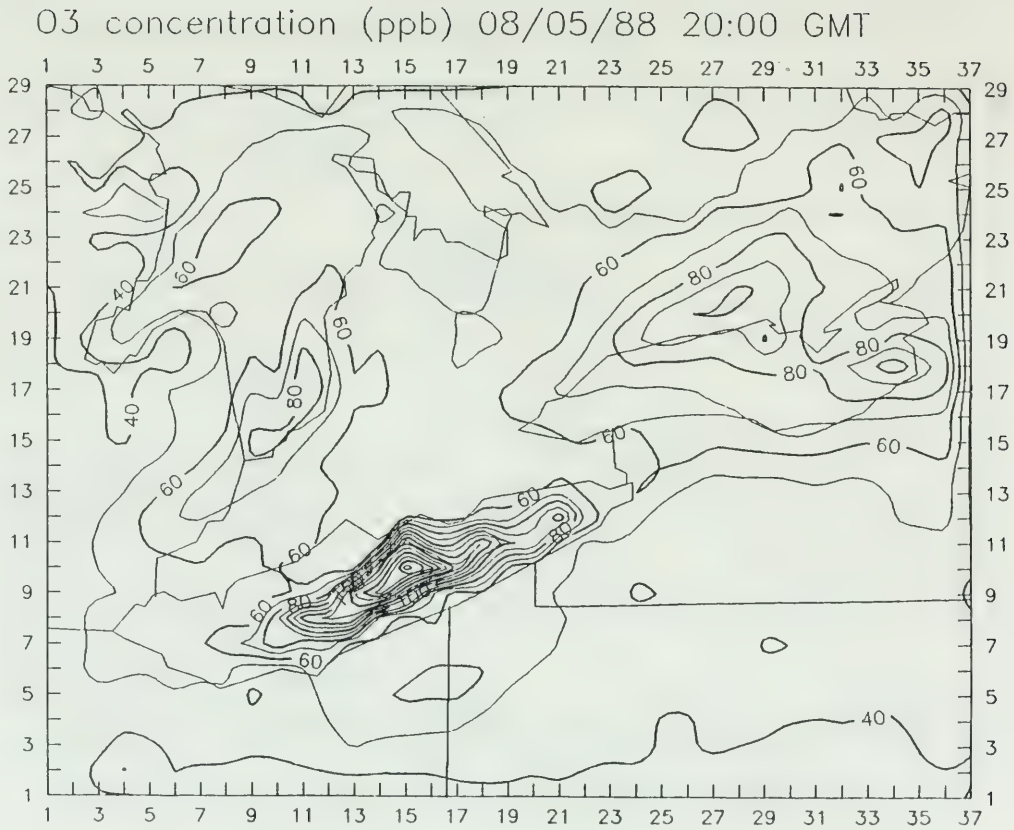

03 concentration (ppb) 08/05/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
40
60
80
100

Figure 20.

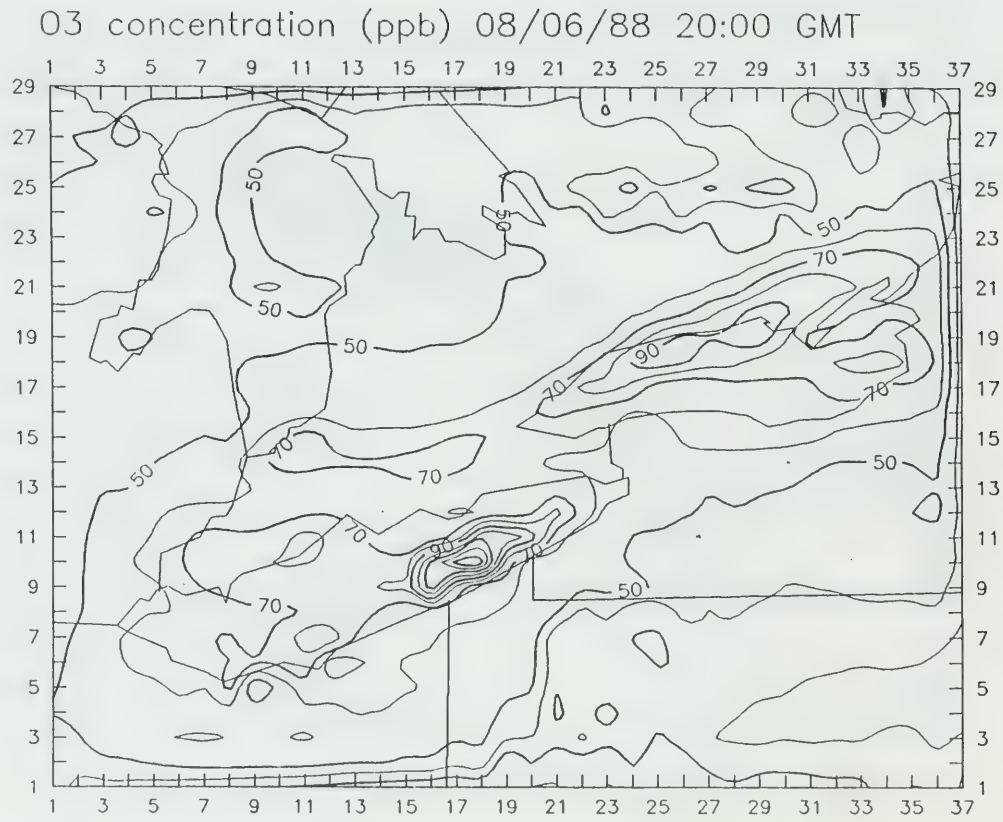

O3 concentration (ppb) 08/06/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
0
50
70
90

Figure 21.

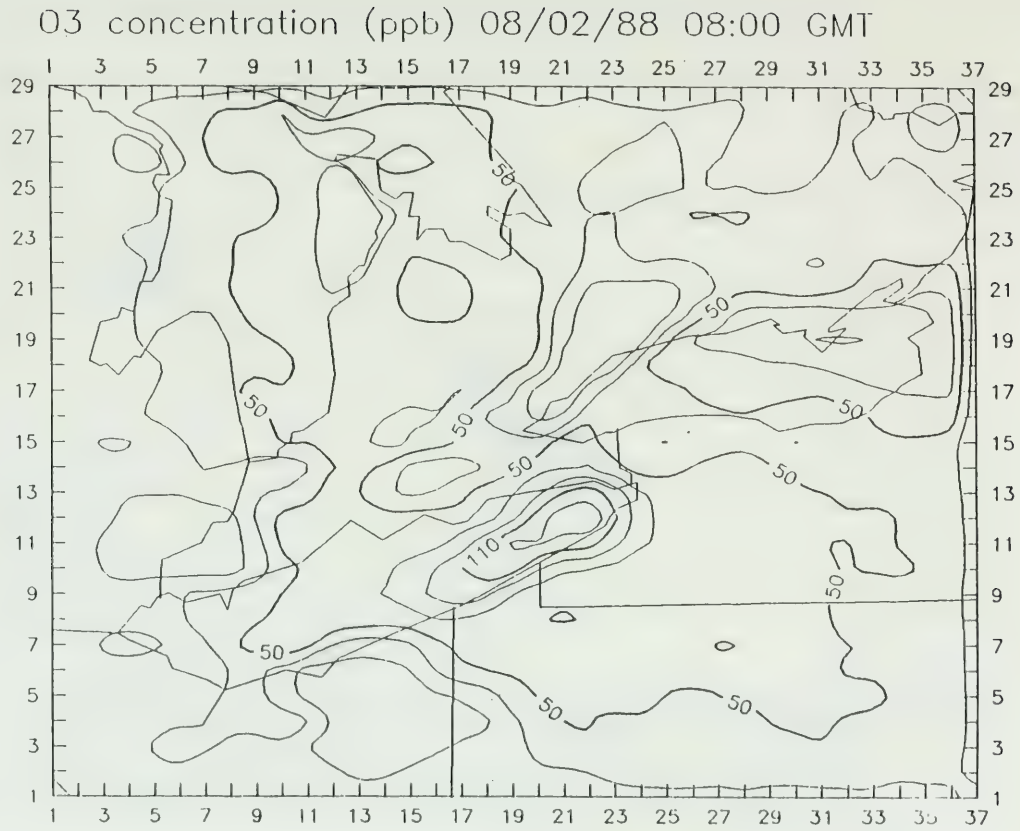

O3 concentration (ppb) 08/02/88 08:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
50
110

Figure 22.

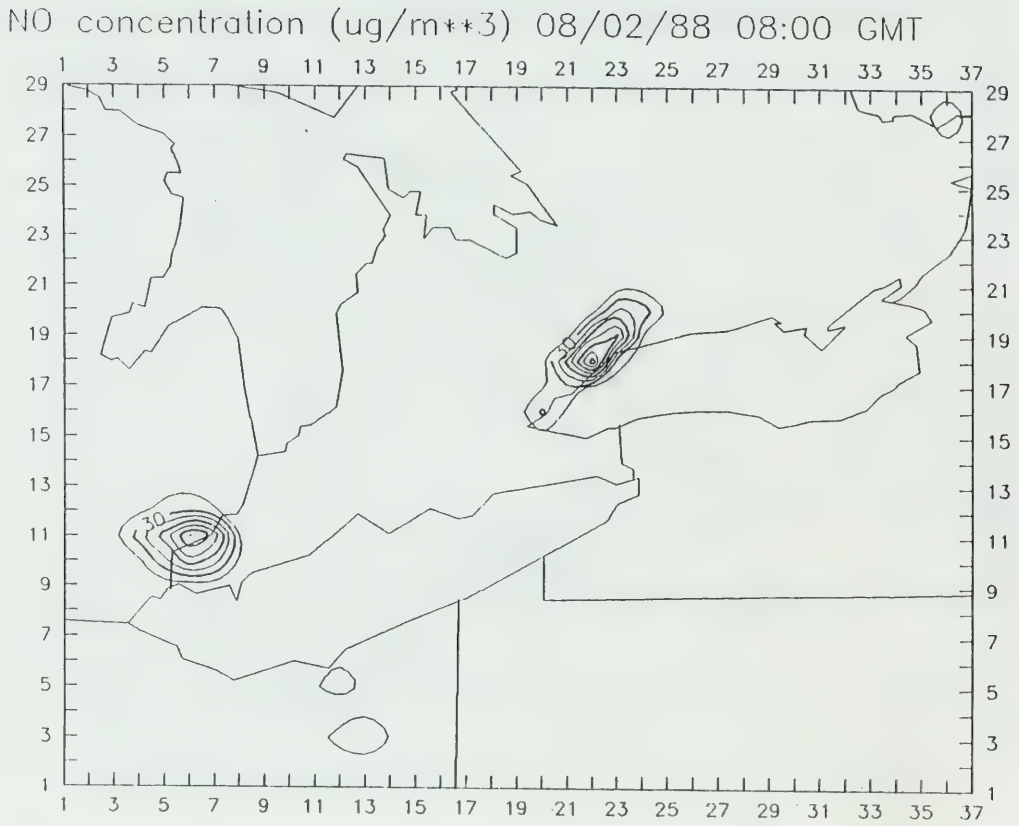
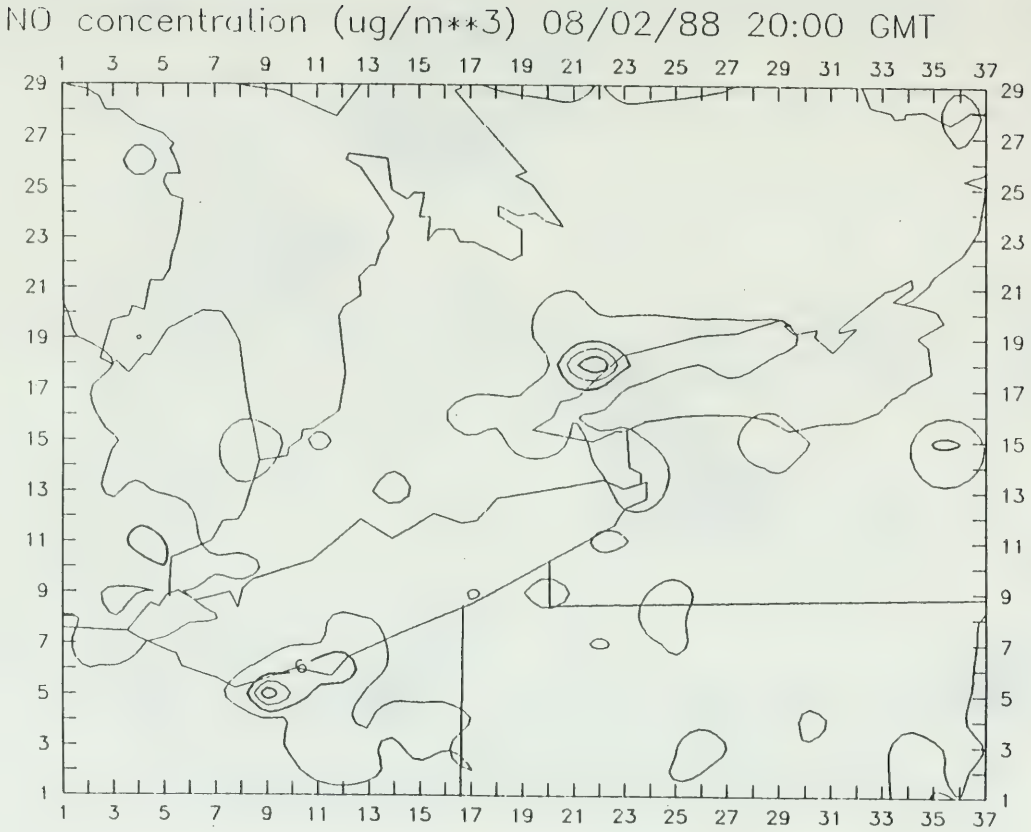

NO concentration (ug/m**3) 08/02/88 08:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
30
Contour interval 20

Figure 23.



contour interval 5

Figure 24.

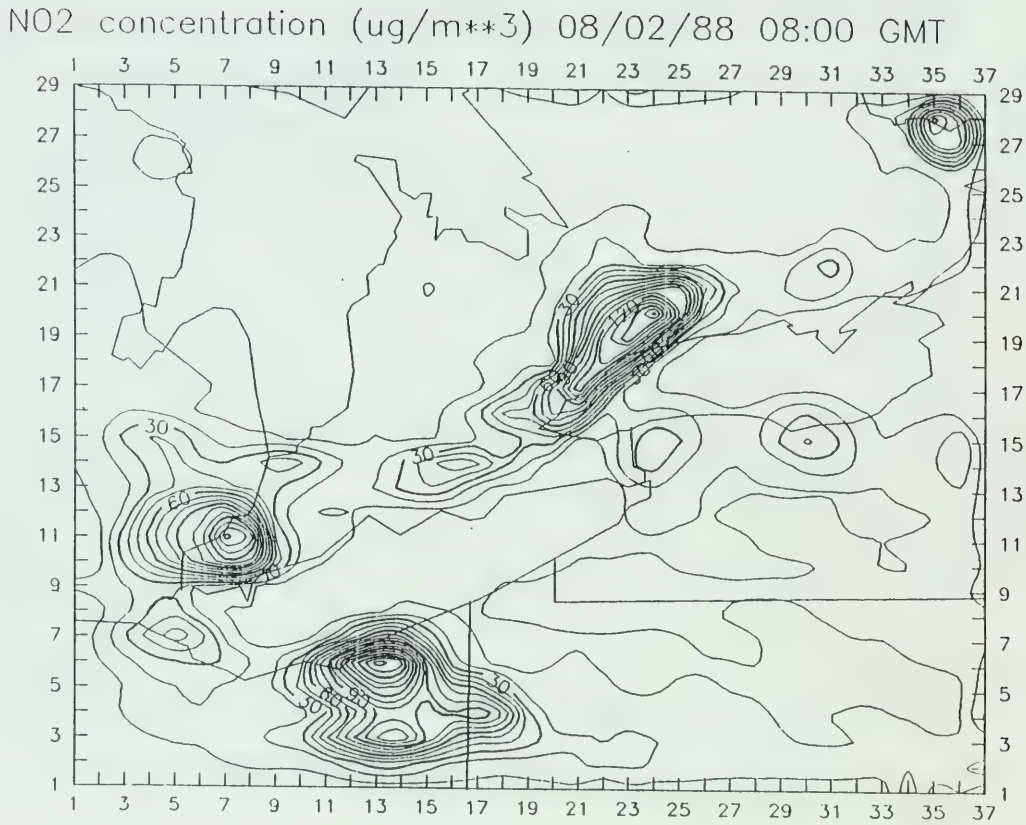

NO2 concentration (ug/m**3) 08/02/88 08:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
30
60
90
120
150

Figure 25.

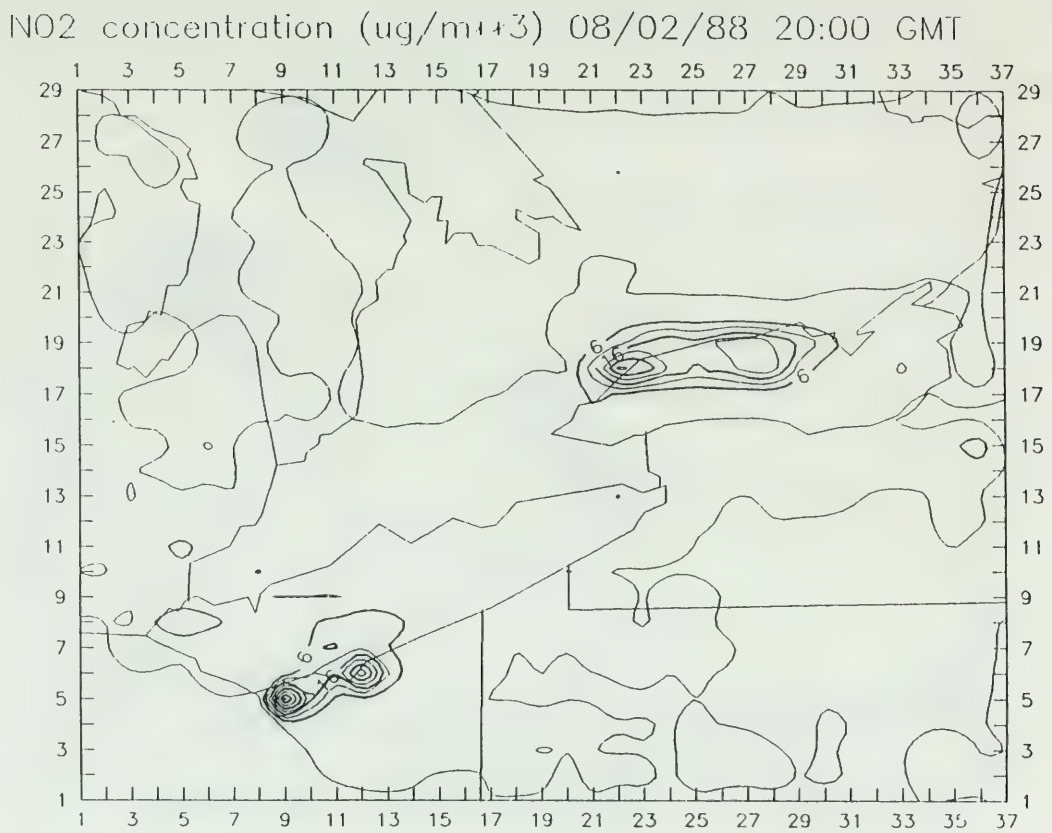

NO2 concentration (ug/m**3) 08/02/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
6
0

Figure 26.

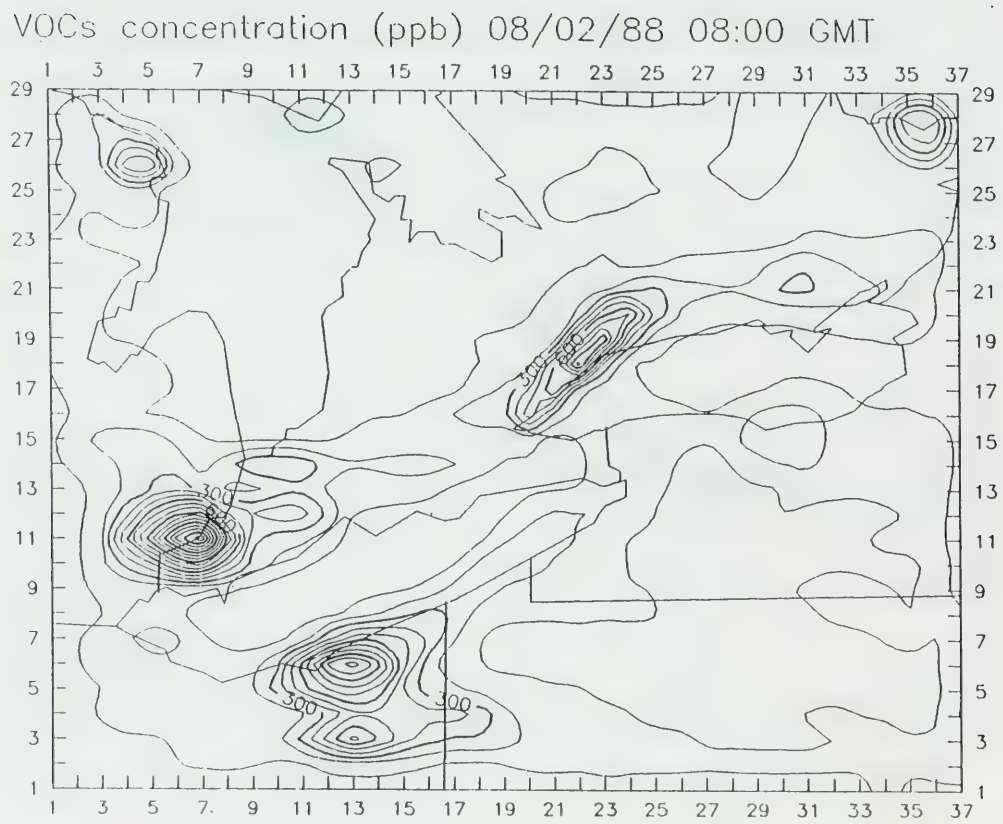

VOCs concentration (ppb) 08/02/88 08:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
300
300
300
300

Figure 27.

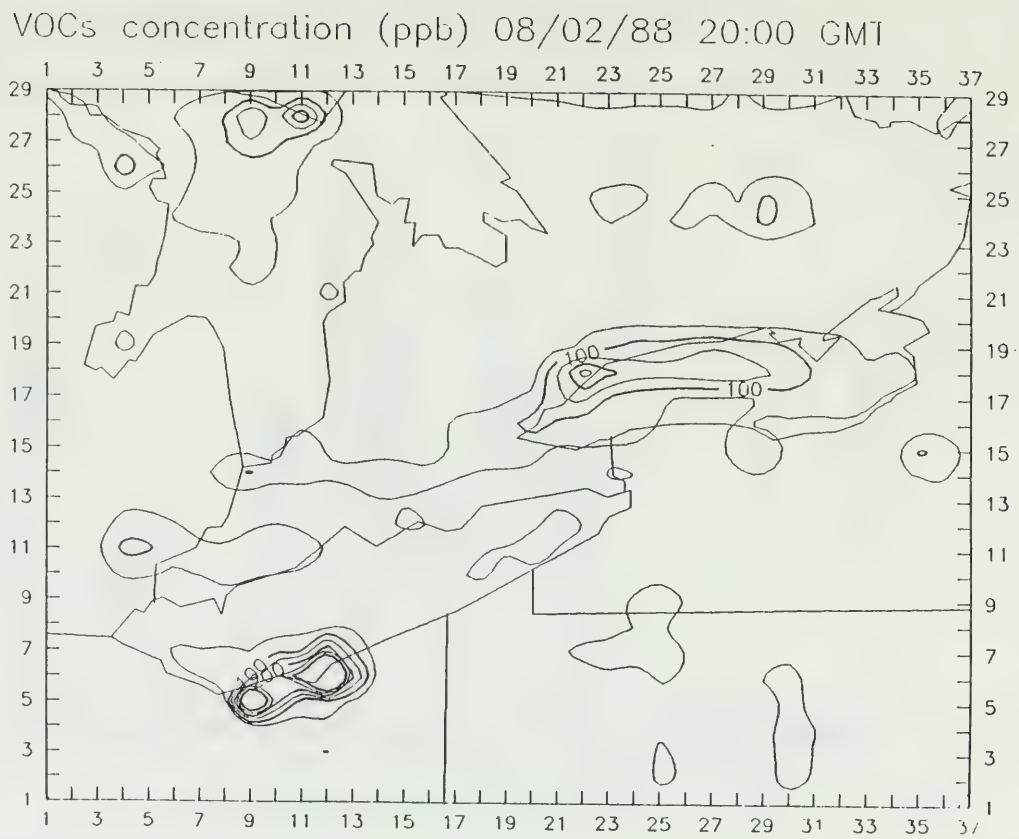

VOCs concentration (ppb) 08/02/88 20:00 GMT
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 31 33 35 37
29 27 25 23 21 19 17 15 13 11 9 7 5 3 1
0
100
100
100

Figure 28.

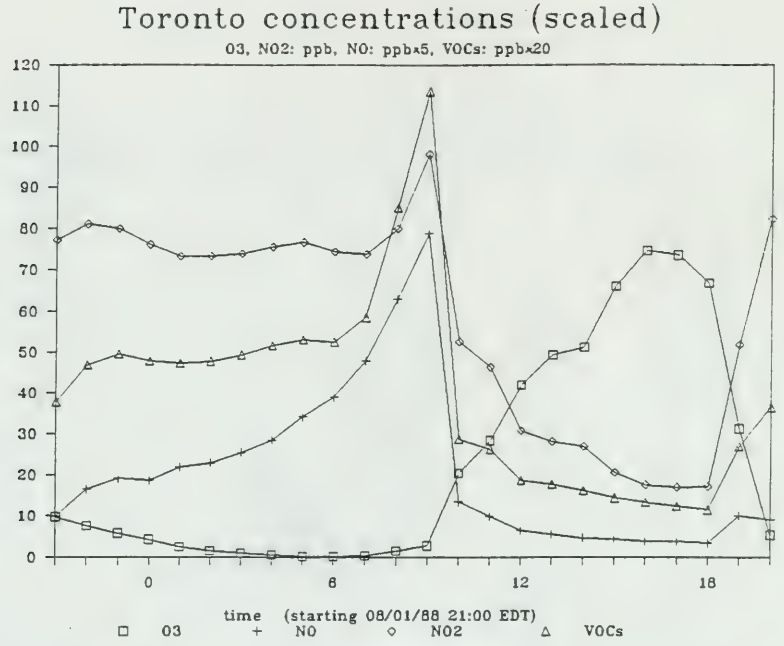


Figure 29.

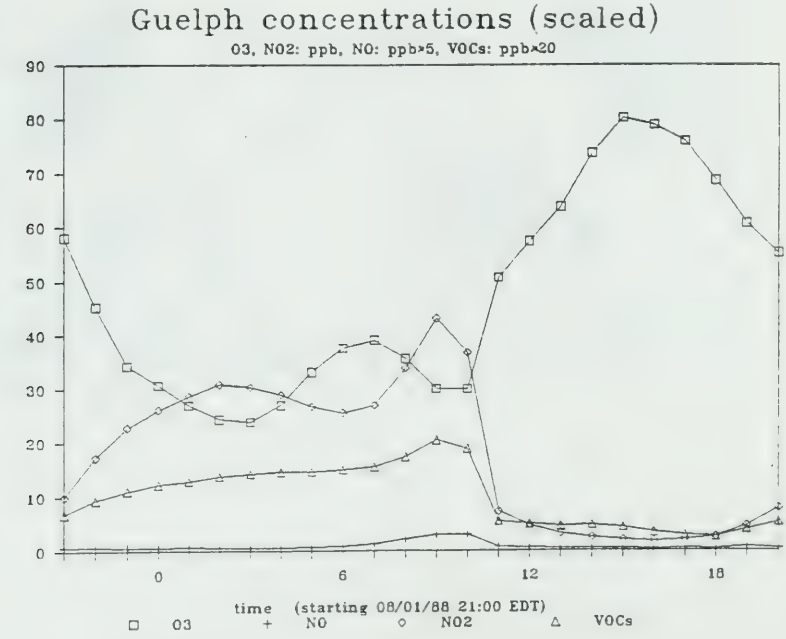


Figure 30.

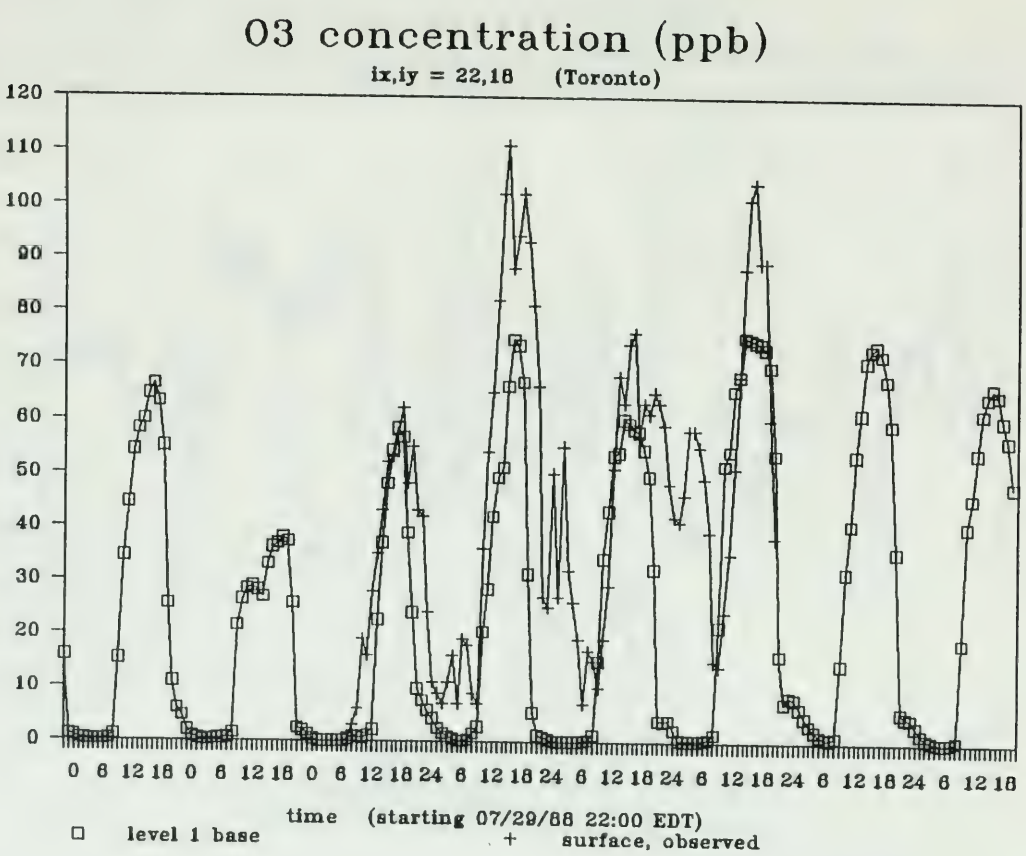

03 concentration (ppb)
ix,iy = 22,18 (Toronto)
120
110
100
90
80
70
60
50
40
30
20
10
0
0 6 12 18 0 6 12 18 0 6 12 18 24 6 12 18 24 6 12 18 24 6 12 18 24 6 12 18 24 6 12 18
time (starting 07/29/88 22:00 EDT)
level 1 base
surface, observed

Figure 31.

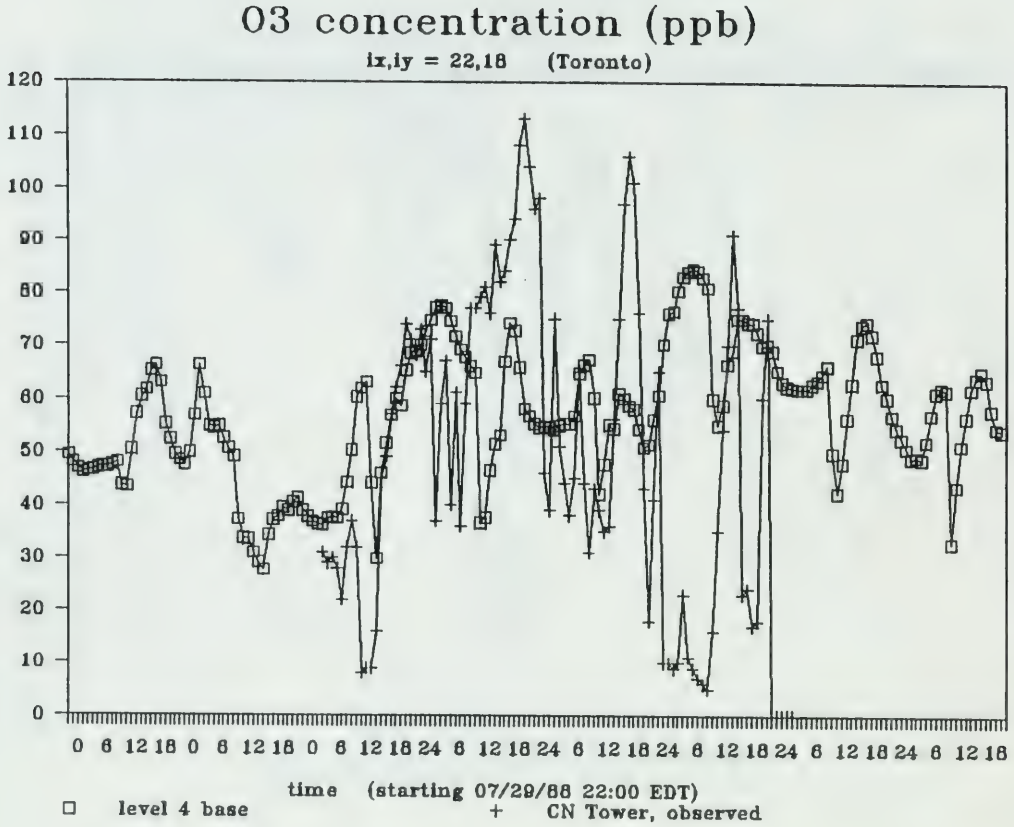

O3 concentration (ppb)
ix,iy = 22,18 (Toronto)
120
110
100
90
80
70
60
50
40
30
20
10
0
0 6 12 18 0 6 12 18 0 6 12 18 24 6 12 18 24 6 12 18 24 6 12 18 24 6 12 18
time (starting 07/29/88 22:00 EDT)
level 4 base
CN Tower, observed

Figure 32.

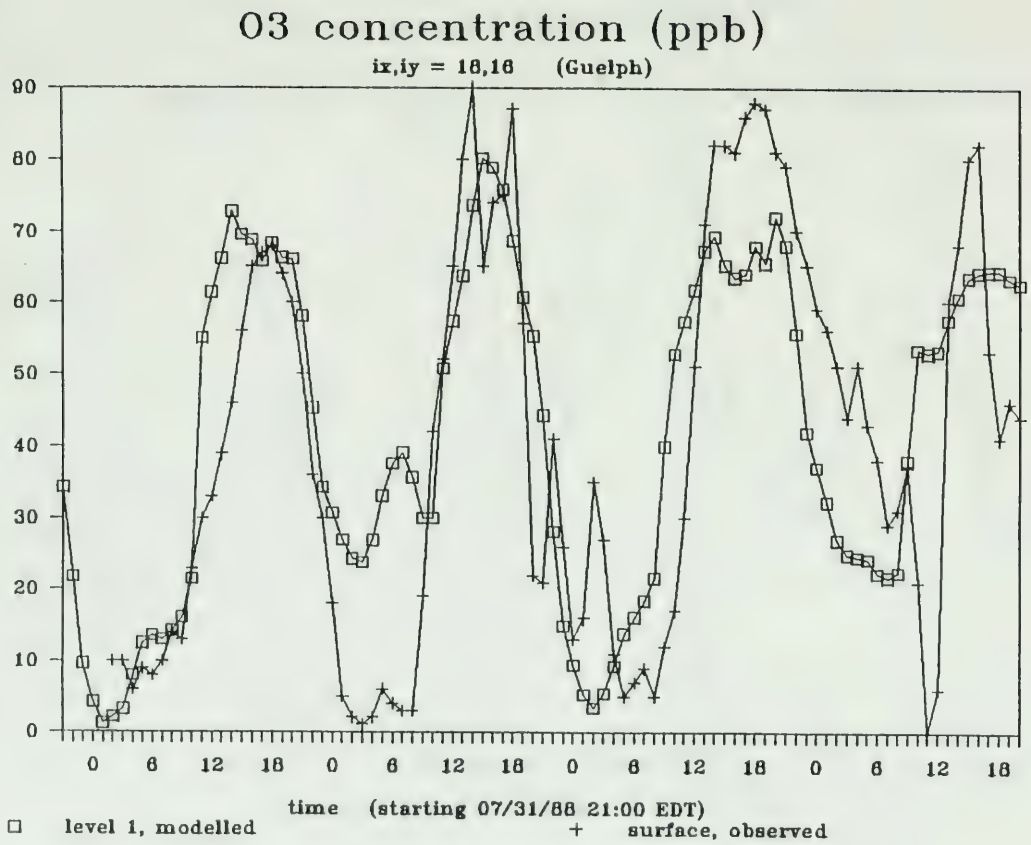

O3 concentration (ppb)
ix,iy = 16,16 (Guelph)
90
80
70
60
50
40
30
20
10
0
0 6 12 18 0 6 12 18 0 6 12 18 0 6 12 18
time (starting 07/31/88 21:00 EDT)
level 1, modelled
surface, observed

Figure 33.

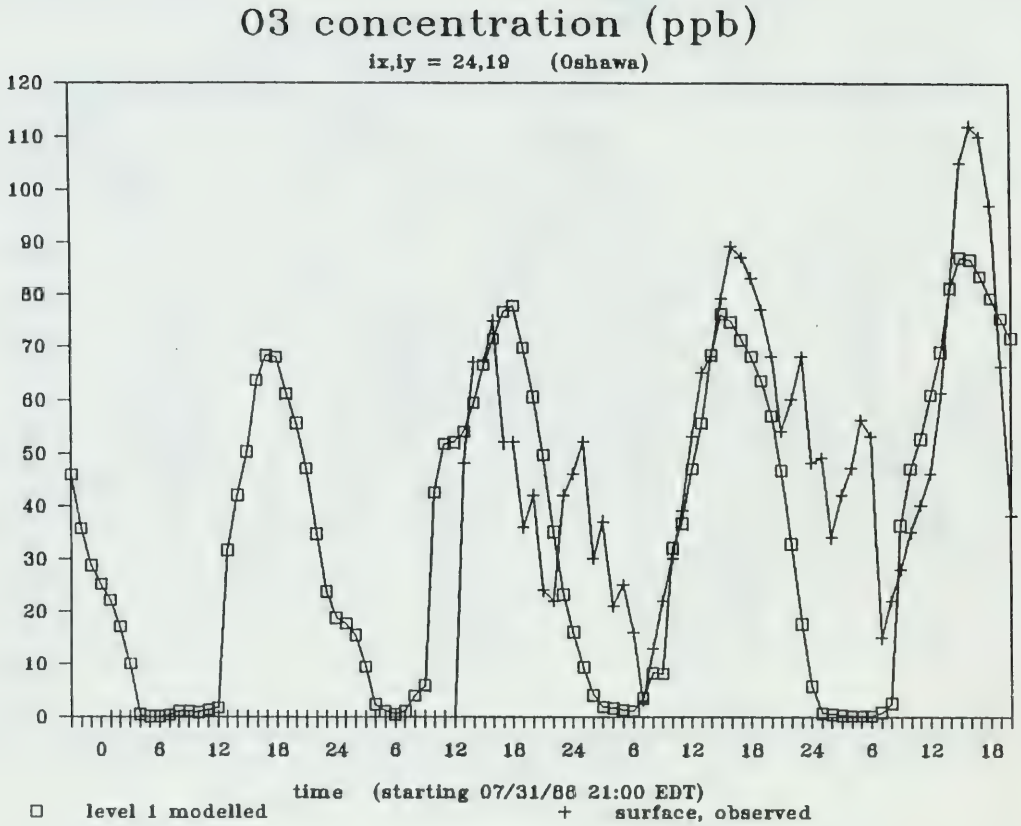

03 concentration (ppb)
ix,iy = 24,19 (Oshawa)
120
110
100
90
80
70
60
50
40
30
20
10
0
0 6 12 18 24 6 12 18 24 6 12 18 24 6 12 18
time (starting 07/31/88 21:00 EDT)
□ level 1 modelled
+ surface, observed

Figure 34.

APPENDIX A

Paper presented at the Technology Transfer Conference,
on November 25-26, 1991 in Toronto

APPENDIX A

THE DEVELOPMENT OF A LONG RANGE TRANSPORT MODEL WITH A NESTED FINE RESOLUTION GRID

by

M. Niewiadomski, The MEP Company, Markham, Ontario L3R 9T2

1. INTRODUCTION

Two existing numerical models, GESIMA, a mesoscale, non-hydrostatic meteorological model developed at the GKSS Forschungszentrum in Geesthacht, Germany and the long range transport Acid Deposition and Oxidant Model (ADOM) have been enhanced, adapted and interfaced to obtain a nested modelling system for the simulation of the transport, chemical transformation and deposition of a wide range of atmospheric pollutants.

The system described here is best suited to simulate the distribution of pollutants with a horizontal resolution of 5 to 20 km. A test run of the system for the Toronto area was carried out in a domain of 340 x 340 km with horizontal resolution of 20 km. A new series of simulations, with the same resolution, is currently being performed in a domain of 700 x 500 km covering most of Southern Ontario.

The resolution and the size of the domain place this system in the mesoscale, i.e. between the urban scale air quality models and the large scale models of long range transport of atmospheric pollutants (LRTAP). A mesoscale modelling capability is necessary to address the urban NOx/VOC issue if an understanding and eventual controlling of the precursor emissions is to be achieved. This approach is also required and to quantify the subgrid scale variability of pollutant concentrations simulated by the LRTAP models.

The modelling system developed in this study involves the interrelation of three main parts: the large scale ADOM, GESIMA, and the mesoscale version of ADOM. The programs interfacing these three parts are also an important part of the system. The interactions between these system components are schematically represented in Figure 1.

The original large scale version of ADOM uses meteorological fields generated by the Canadian Meteorological Centre (CMC) spectral diagnostic model. The mesoscale ADOM requires three-dimensional fields of meteorological parameters like horizontal and vertical wind velocity, temperature, humidity, turbulent diffusion parameters etc., with much finer horizontal resolution. Such fields are provided in this project by GESIMA. The role of the large scale ADOM, is to provide the initial and boundary conditions for the mesoscale simulations.

For a brief description of the main features of the system components, see Niewiadomski (1990). More details can be found in the original papers on ADOM (Scire et al., 1986; Venkatram et al., 1988) and GESIMA (Kapitza, 1987; Kapitza and Eppel, 1987; Jacob et al., 1990 and Mengelkamp, 1991).

2. THE NESTING SCHEME

For simulations periods longer than, say, one day, a mesoscale model must receive information of the development of the modelled fields outside its domain. This is achieved by "nesting" the mesoscale model inside an outer model operating in a much larger domain but with a more coarse resolution. In the system described here the outer model for GESIMA is the CMC diagnostic model, which also provides the meteorological fields for the large scale ADOM. The mesoscale ADOM is nested in the large scale version operating on the same grid as the CMC model.

In this system the mesoscale domain covers a specified number of cells of the large scale grid. The large scale data from these cells, and those adjacent to the mesoscale domain, can be interpolated in space and, if necessary, in time and then passed to the mesoscale model.

The mesoscale ADOM receives information from the outer model through time dependent boundary conditions. Similar time dependent boundary conditions are used for some parameters in GESIMA, but for the main fields (wind, temperature and humidity) a technique of the Newtonian relaxation or "nudging" is used.

The concept of nudging (Hoke and Anthes, 1976; Stauffer and Seaman, 1990; Seaman and Cole, 1991) involves the introduction of additional, artificial tendency terms to the prognostic equations, which force the solution of the mesoscale model toward the observed, or modelled, large scale conditions. This approach is used to combine the fine scale variability with the large scale tendencies which cannot be simulated by the mesoscale model itself, and seems to be more efficient and reasonable than introducing those tendencies by means of the time dependent boundary conditions alone.

These artificial tendencies - the nudging terms, applied at each time step, are proportional to the difference between the values of large scale field at given grid point (interpolated from the results of the outer model) and the actual solution of the mesoscale model. The coefficient of proportionality - the nudging coefficient, can be a function of height and has values of the order of 0.0001/sec.

Note that the described above nesting scheme represents so called one-way nesting, i.e. the results of the mesoscale simulations do not influence the large scale models. This allows all components of the system to be run separately and to simulate several emission/pollution scenarios using the same meteorological fields.

3. SIMULATION OF THE HIGH OZONE EPISODE (August 1 - 4, 1988)

This section gives the details of a test run of the system. The episode for this study, August 1 - 4, 1988 was chosen because of the high ozone concentrations observed at that time in Southern Ontario, and the availability of the results of the large scale ADOM simulation and the observational data.

Some results of this simulation concerning the time evolution of the ozone concentrations in Toronto and its areal distribution in the whole domain are presented and discussed in Section 4.

The large scale ADOM is routinely run on a 33 x 33 grid based on a polar stereographic projection with nominal horizontal resolution of 127 km (true at 60° N). That domain covers most of eastern North America. The same grid is used in the CMC spectal model.

In this simulation, the 'nested' grid of GESIMA and mesoscale ADOM covers 9 cells of the large grid, including the Toronto cell and the 8 cells around it. Thus, the mesoscale domain extends over an area of about 120,000 km² with Metropolitan Toronto area located about 25 km south of its centre. The domain is divided into 17 x 17 mesoscale cells resulting in a horizontal resolution of about 20 km.

The basic vertical structure of the large scale ADOM, with 12 variable depth layers has been retained for the mesoscale version of the model. The same structure was adopted for the GESIMA simulations. The tops of the ADOM layers are located at 56.2, 135.8, 250.7, 416.3, 655.3, 1000.0, 1497.2, 2214.5, 3249.2, 4741.6, 6894.5, and 10000.0 metres above the ground level. The vertical resolution of the upper layers of ADOM is too coarse for GESIMA, and therefore the 4 top layers of ADOM were split into two layers. In effect, 16 rather than 12 vertical layers are used in GESIMA. The GESIMA/ADOM interface averages the data from those split layers before using them in appropriate layers of ADOM.

GESIMA was run for a period of 96 hours starting on August 1, 1988 at 00:00 GMT (July 31, 20:00 EDT) and a time step of 45 sec was used throughout this period.

The large scale ADOM was not run under this project. The output files, from a previous simulation for the same period were used. These files together with the output of GESIMA, were processed by the interfacing programs and provided the input data for the mesoscale ADOM simulations.

Since the mesoscale ADOM requires GESIMA output data, the ADOM run started one hour later then that of GESIMA, at 01:00 GMT, on August 1, 1988 and continued for 95 hours.

4. RESULTS

The time evolution of the ozone concentration in the Toronto cell of the mesoscale model is compared with observations in Figure 2.

The times of maximum and minimum modelled concentrations coincide with those observed at the surface in Toronto (except for a secondary peak in observed concentrations during the early morning of Aug 4 which is not reflected in the model results).

The values of the modelled ozone concentrations are also in fairly good agreement with the observed ones, although the model does not predict the highest measured concentrations (e.g. 112 ppb observed in Toronto on Aug. 2 at 14:00 EDT versus 68 ppb modelled). These discrepancies can be partly attributed to a significant area and depth represented by an ADOM cell, compared to the point measurements. Comparisons made for several other locations with available surface measurements of ozone concentrations yielded similar results.

Examples of the areal distribution of ozone and nitrogen oxides are shown in Figure 3. While the NO_x distribution is dominated by strong area and point source emissions in the Toronto area and the ozone is distributed more evenly, both fields display a pronounced horizontal variability impossible to simulate with a large scale - coarse resolution models.

5. CONCLUSIONS

A mesoscale modelling system for transport, chemical transformation and deposition of atmospheric pollutants has been designed, programmed and tested in one case study over Southern Ontario.

The system is capable of simulating the distribution of various air pollutants with a spatial resolution of 20 km or less. It can detect local effects in this scale that are impossible to simulate with large scale models like the original version of ADOM.

A preliminary analysis of the simulation of the early August 1988 high ozone episode over Southern Ontario, showed reasonably good agreement of the model results with observations.

A case study of the same episode using a slightly modified model, over a large domain covering most of Southern Ontario is currently underway.

6. ACKNOWLEDGEMENTS

The author would like to thank Drs. P.K. Misra and C. Fung of the Ontario Ministry of the Environment, Dr. D. Eppel of GKSS, and Mr. L. Shenfeld of The MEP Company for their assistance in this study.

7. REFERENCES

Hoke J.E. and R.A. Anthes (1976) The initialization of numerical models by dynamic initialization technique. Mon. Wea. Rev. 104, 1551 - 1556.

Jacob D., W. Koch, L., Levkov and D.P. Eppel (1990) Cloud formation within a sea-breeze circulation system. Proc. 4-th Conf on Mesoscale Processes, Boulder, Colorado June 25-29, 1990.

Kapitza H. (1987) Das dynamische Gerust eines nicht-hydrostatischen Mesoskalen-Modells der atmospharischen Zirculation. GKSS 87/E/35.

Kapitza H. and D. Eppel (1987) A 3-D Poisson solver based on conjugate gradients compared to standard iterative methods and its performance on vector computers. J. Comput. Phys. 68, 474 - 484.

Mengelkamp H. T. (1991) Boundary layer structure over an inhomogeneous surface: simulation with a non-hydrostatic mesoscale model. Boundary Layer Meteorology, in press.

Niewiadomski M. (1990) Mesoscale and long range transport models are combined to model pollutants from local and distant sources. Proc. Technology Transfer Conf. Toronto, November 19 - 20, 1990, 206 - 209.

Scire J.S., F.W. Lurmann, P. Karamchandani, A. Venkatram, R. Yamartino, J. Young and J. Pleim (1986) ADOM/TADAP development program, Vol. 9: ADOM/TADAP user's guide. Report for the Ontario Ministry of the Environment, the Umweltbundesamt (Germany) and Environment Canada by the ERT Company, Newbury Park, California.

Seaman N.L. and C.D. Cole (1991) Application of four-dimensional data assimilation for generating three-day episodic meteorological fields over the Los Angeles basin suitable for air quality modeling. Proc. 7-th Joint AMS/APCA Conference on Applications of Air Pollution Meteorology, New Orleans, Louisiana, Jan. 13-18, 1991, pp 320 - 323.

Stauffer D.R. and N.L. Seaman (1990) Use of four-dimensional data assimilation in a limited-area mesoscale model. Part I: Experiments with synoptic scale data. Mon. Wea. Rev., 118, 1250 - 1277.

Venkatram A., P.K. Karamchandani and P.K. Misra (1988) Testing a comprehensive acid deposition model. Atmospheric Environment 22, 737 - 747.

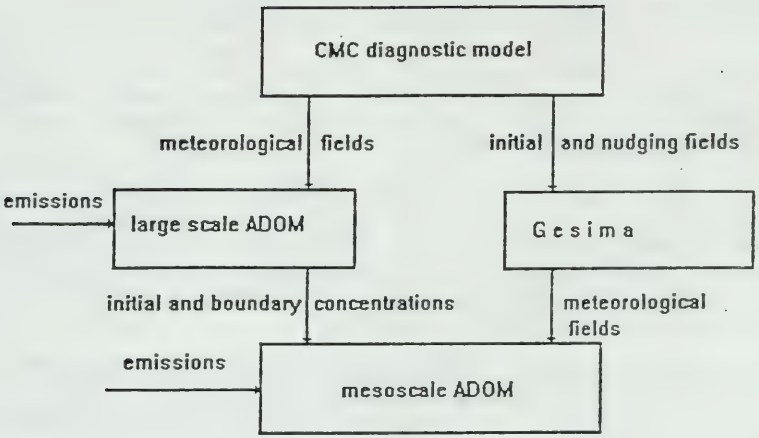


FIGURE 1

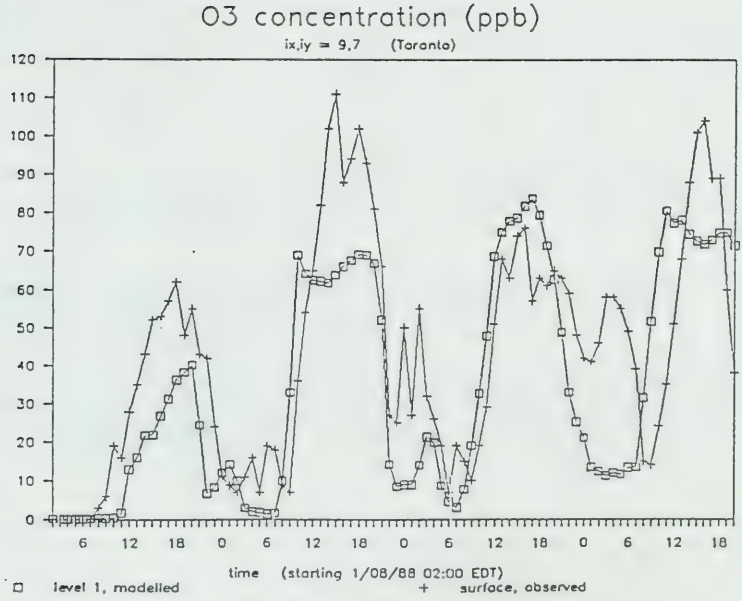


FIGURE 2

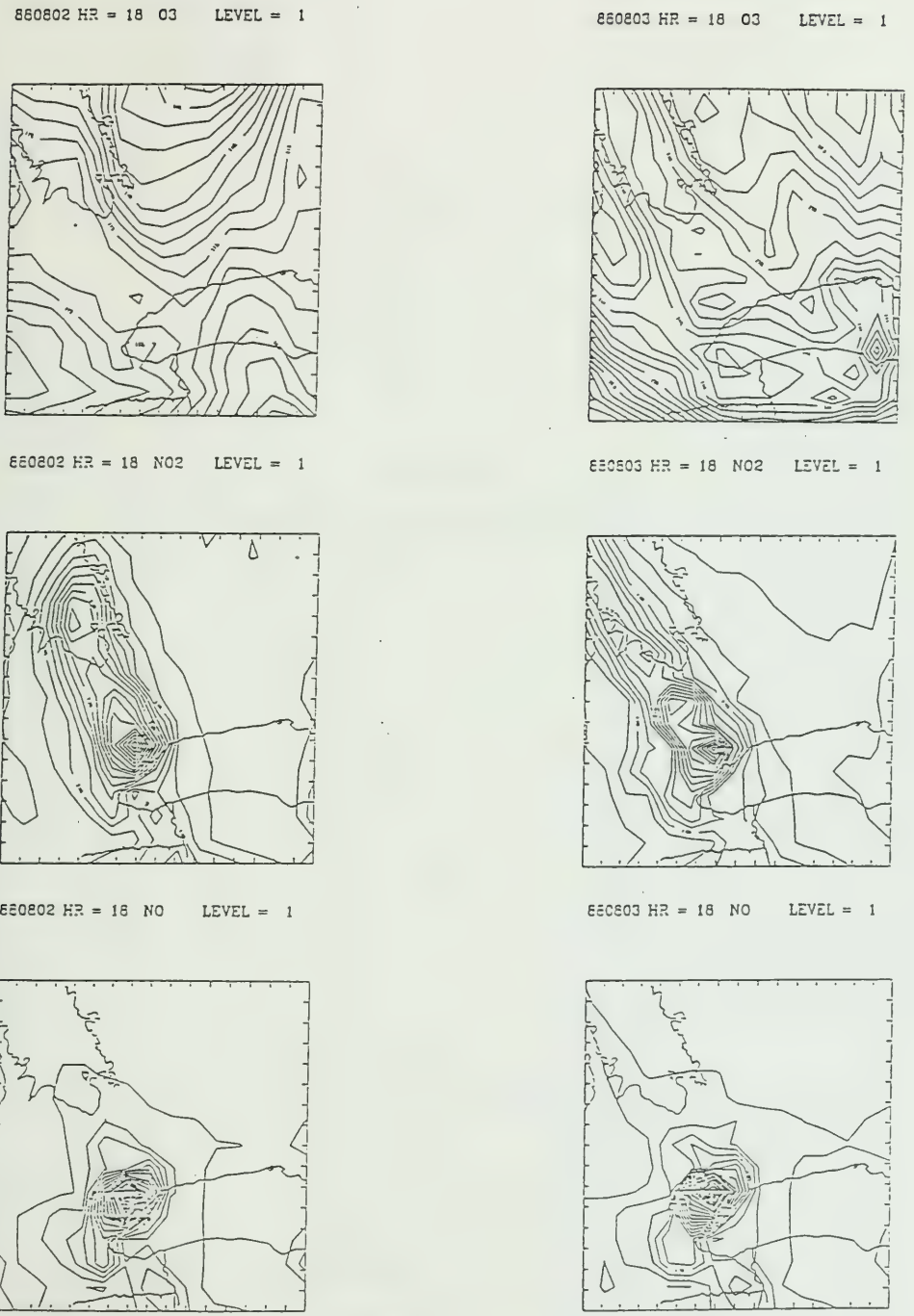


FIGURE 3. Concentrations of O_3, NO and NO_2 ($\mu g/m^3$) in the lowest layer of the model at 2 p.m. EDT (18:00 GMT) on the second and third day of simulation.

APPENDIX B

Description of the Gesima input file

APPENDIX B

Description of the Gesima input file (fort.15)

The general input file is organized in namelists. The file is read by subroutine READD at the beginning of each job. Namelists HOTCOL, SWITCH and AEROSO are also read from MAIN. Only those three namelists are read in the case of a restart (continuation) run, thus only the parameters belonging to those namelists can change values after the beginning of an initial job.

The basic structure of the input file and most of the input parameters originate from the original, GKSS version of the model. Some of them are redundant for the present application, but have been retained in the input file for the sake of compatibility with original model and therefore require a value to be provided in the input file. Other parameters may require specific
values for this study. Such values are provided below, where applicable. For other parameters either a recommended value (for the 37 x 29 grid with 20 km resolution and the August 1988 simulation) is given or an exemplary value from a recent run.

1. Namelist HOTCOL

This namelist contains the main control parameters of the model. For the regular simulations, the model should be run for one or more full hours, beginning on IHR0 and ending at IHR1 on the same date. Other simulation time parameters are of secondary importance. The length of the time step DELTAT should be chosen so that an integer number of steps is made in one hour. The description of input parameters is given below.

Initial/restart run indicator:

IFHOTS	= 0	for an initial run
	= 1	for a continuation run

Intervals (in seconds) of calls to SAFETY and writing a restart file:

INCHOT	= 3600	(exemplary value)

Time step in seconds:

DELTAT	= 45.	(recommended value, see comments on DELTAT above)

Intervals (in seconds) of calls to PRINTT and writing output files:

INCOUT	= 21600	(exemplary value)

Intervals (in seconds) of calls to MONITO and writing auxiliary output:

IFMONI	= 20000	(exemplary value)

Maximum total time of simulation:

TIMAX	= 10000000	(any large number)

Setting TIMAX to lower values is useful for short test runs. The simulation will stop after reaching TIMAX, even if IHR1 is not reached.

INRAD	= 2	(any value - not used in this version)
IFTIM	= 0	(required value - TIMSTP not called, for IFTIM = 1 variable timestep is internally computed).
IFSTAT	= 0	(required value, IFSTAT = 1 means 'static' simulation)

Filter parameters:

FILX	= 0.025	(recommended value)
FILY	= 0.025	(recommended value)
FILZ	= 0.00	(recommended value)

Smoothing parameters

SMCO	= 0.0	(any value - not used in this version)
SMCOM	= 0.0	(any value - not used in this version)

Geostrophic wind parameter:

KGEO	= 10	(recommended value, geostrophic wind is assumed as equal to the nudging wind at appropriate level for all levels above KGEO and to the nudging wind at KGEO below that level)

Initial and final hour of simulations (GMT):

IHR0	= 0	(exemplary value)
IHR1	= 6	(exemplary value)

First hour (GMT) for which the nudging data should be read from units 91 and 41 rather than 81 and 21:

IHR91	= 24	(exemplary value)

```
IFRELA          = -1            (Value required for a regular run,
                                 other values can be used for some
                                 special, mostly obsolete cases,
                                 for details see subroutines
                                 RDBC and RDBCI)

IDAY            = 1             (any value less then 10, other
                                 values can be used for some
                                 special, mostly obsolete cases,
                                 for details see subroutines RDBC
                                 and RDBCI)

Intervals (in seconds) of calls to WRTAPE and writing ADOM output
file:
INTAP           = 3600          (recommended value)

Nudging coefficients for humidity, temperature and wind, NZ+2
values each:
QNUD            = 18*1.E-4      (recommended values)
TNUD            = 18*1.E-4      (recommended values)
UNUD            = 18*1.E-4      (recommended values)

Model version:
VRSION          = 'GES/ENE'     (exemplary value, not important in
                                 this application)

Start of simulation date:
ISTART          = 880806        (exemplary value)

Julian time (day, GMT hour) of the start of simulation
IJULS           = 21900         (exemplary value)

End of simulation date:
IIEND           = 880806        (exemplary value)

ADOM output file append switch:
ITAPPE          = 0             if a new ADOM output file (fort.32)
                                is to be written.
                = 1             If ADOM output is to be appended
                                to the results of a previous run.
```

2. Namelist GEOMET

This namelist contains the grid definition and some auxiliary parameters. Only the vertical grid data are meaningful for this application. The vertical layers correspond to those of ADOM, with 4 uppermost layers split in two to enhance the resolution. The additional level at the top (NZ+1) is at the same distance from the top as the level NZ-1).

Horizontal grid (NX+3 values in x direction and NY+3 in y direction):

XE	= 40*0.	(any values, grid redefined in subroutine READD)
YN	= 32*0.	(any values, grid redefined in subroutine READD)

Vertical grid (tops of each layer in m, NZP+2 values), required values:

ZW = 0.,56.1983,135.8103, 250.6563, 416.3205,655.2896, 1000., 1497.2413, 2214.5072, 2731.8316, 3249.1559,3995.3912, 4741.6265, 5818.0661, 6894.5056, 447.2528, 10000., 11552.7472

Height of the bottom and top of the domain (m):

HBOT	= 0.	(required value)
HTOP	= 10000.	(required value)
RTOP	= 25000.	(any value - not used in this version)

Height of topography (in m, (NX+3)*(NY+3) values):

ZGNE	= 1280*0.	(any values, topography redefined in subroutine RTOPO)

Land use category, (NX+2)*(NY+2) values:

LWTYP	= 1209*8	(any values - not used in this version)

3. Namelist PARMET

This namelist contains mostly physical parameters, which do not change during the simulation.

Average latitude of the domain (deg):

PHI	= 44.	(exemplary value)

Start of simulation in days from the beginning of spring

DAY	= 130.	(exemplary value)

Mean cloud coverage:

COV	= 0.0	(any value - not used in this version)

```
Sea surface temperature:
TNSEA          = 286.          (any value - not used in this
                                version)

Pressure solver parameters:
ITMAX          = 200           (recommended value)
RESMAX         = 2.E-04        (recommended value)
RESM2          = 2.E-2         (recommended value)
RESFAC         = 4.            (recommended value)

Geostrophic wind components (m/s):
UGEO           = 4.0           (any value - not used in this
                                version)
VGEO           = -2.0          (any value - not used in this
                                version)

Reference potential temperature profile (NZ+2) values:
THET0          = 18*290.       (recommended values)

Reference sea level pressure (Pa):
PSEAL          = 1.E5          (recommended value)


Reference sea level temperature (K):
T0             = 290.          (recommended value)

Reference sea level potential temperature (K):
THSEAL         = 290.          (recommended value)

Reference temperature profile parameter:
GAMMA          = 0.6           (recommended value)

Parameters for test topography runs - see subroutine READD)
AMPL           = 200.,         (any value - not used in this
                                version)
AMPL2          = 300.,         (any value - not used in this
                                version)
WIDTH          = 10000.,       (any value - not used in this
                                version)
WIDTH2         = 25000.,       (any value - not used in this
                                version)
XCENT          = 75000.,       (any value - not used in this
                                version)
YCENT          = 150000.,      (any value - not used in this
                                version)

Height of the damping layer
ZDAMP          = 6894.5056     (any value, damping layer defined
                                by IFDAMP)
```

```
Damping coefficient:
DAMFAC          = 0.024         (recommended value)

A small number:
SMALL           = 1.E-30        (recommended value)

Implicit diffusion parameter:
TDIF            = 1.50          (recommended value)

Tracer parameters, 3 values each:
XTRAC = 1000., 5000, 10000.     (any values - not used in this
                                 version)
YTRAC = 1000., 3000., 3000.     (any values - not used in this
                                 version)
ZTRAC =   10.,  100., 1500.     (any values - not used in this
                                 version)

Permutation parameter, 24 values (required values):
IPERM = 1,1,1, 0,0,1, 1,1,0, 0,1,0, 1,0,1, 0,1,1, 1,0,0, 0,0,0
```

4. Namelist SWITCH

This namelist contains switch variables which activate or deactivate various options of the model. Usually only one choice is possible for this application. The purpose of each switch is given below along with the settings required for this study. For other possible values of the switches and their meanings see the appropriate subroutines.

Note that even that this namelist is read also at the beginning of restart jobs, and the setting of switches can be changed, some of such changes may introduce inconsistencies in the model and lead to the execution time errors.

```
Inflow and outflow boundary condition switches for temperature,
wind, vertical velocity and humidity:
IFTINF          = 1             (required value)
IFTOUT          = 1             (required value)
IFUINF          =-1             (required value)
IFUOUT          =-1             (required value)
IFWINF          = 1             (required value)
IFWOUT          = 1             (required value)
IFQINF          = 1             (required value)
IFQOUT          = 1             (required value)

Nudging switches for temperature, humidity and wind (1: ON,
0: OFF):
IFNUT           = 1             (required value)
IFNUQ           = 1             (required value)
IFNUU           = 1             (required value)
```

```
Velocity initialization switches:
IFINUW          = 1             (required value)
IFINFB          = 1             (required value)
IFINFL          = 1             (required value)

Thicknes of the damping layer (IFDAMT uppermost levels):
IFDAMT          = 4             (recommended value)

Surface wetness switch:
IFSWET          = 0             (required value)

Land use data switch:
IFLWTY          = 0             (required value)

Temperature initialization switches:
IFINTP          = 0             (required value)
IFTETA          = 1             (recommended value)

Reference temperature profile switch:
IFPROF          = 2             (required value)

Filter switch (0,3 or 5 point filtering):
IFFILT          = 5             (required value)

Topography type switch:
IFTOPO          = 0             (required value)

Turbulence parameterization switch:
IFDIFF          = 2             (required value)

Hydrostatic pressure switches:
IFHYUP          = 1             (required value)
IFHYTO          = 1             (required value)
IFHYGR          = 1             (required value)

Auxiliary output switch:
IFCHEC          = 0             (recommended value)

Coriolis force switch:
IFCORI          = 0             (recommended value)

Top and bottom boundary condition switches:
IFTBOT          = 3             (required value)
IFTTOP          = 0             (required value)
IFUBOT          = 3             (required value)
IFUTOP          = 0             (required value)
IFCBOT          = 3             (required value)
IFCTOP          = 1             (required value)

Humidity simulation switch:
IFHUMI          = 1             (required value)
```

Cloud module switch:
IFCLOU = 0 (required value)

Surface module switch:
IFSURF = 1 (required value)

Passive tracer switch:
IFPASS = 0 (required value)

Longwave radiation switch:
IFRAD = 0 (required value)

Unit numbers for output files written by subroutine PRINTT,
22 values, (recommended values):
IFOUTP = 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 64,
70, 71, 72, 73, 74, 75, 76, 77, 0, 0,

5. Namelist AEROSO

This namelist contains the assumed CCN profile (variable AERP, NZ values). Since in the present application the cloud module is turned off (IFCLOU=0) the values of AERP are irrelevant. Exemplary values are given below:

AERP = 300,300,300,300,150,150,30,30,30,30,30,30,20,20,10

APPENDIX C

Modifications of Gesima undertaken under Phase II under this project

APPENDIX C

Modifications of Gesima undertaken under Phase II of this project.

C.1 The MAIN program

The new subroutine NUDEV (see Section C.4) is executed just before PRINTT at INCOUT intervals.

Calls to subroutines WRTAP and RLUSE have been replaced by calls to new subroutines WRTAPF (see Section) and RLUSEX (see Section C.8)

C.2 Subroutine INITS

The purpose of this subroutine is to initialize the variables of the surface layer module. In particular, the variable XSOIL contains for each grid cell the 8 surface parameters, computed as averages of values prescribed to several land use classes, weighted by the relative coverage of the given grid cell by those land types (see Section A1.2 of the last year report).

In place of 11 land use classes used in Phase I, the 8 classes of ADOM (water, deciduous forest, coniferous forest, swamp, cultivated, grass, urban and desert) were introduced to Gesima. The surface parameters were assigned to these classes by directly assigning or, in some cases, averaging the values from the appropriate classes of the 19 used in the original Gesima.

Reduction of the number of classes resulted in changes in dimensions of some variables (XWTYP, XSOIL etc.) and in the averaging formula.

Analysis of the code of subroutine SURFW showed, that in some cases two XSOIL surface parameters were used in one statement. For example the product of the diffusion coefficient and the heat capacity XSOIL(i,j,1)*XSOIL(i,j,2) appeared in some statements. Thus, the product of two averages was used where an average of a product would be more appropriate. In order to correct this situation a new variable DIFCAP(NX,NY) - an average product of the diffusion coefficient and the heat capacity, weighted by the coverage of the grid cell by various land use classes is computed in INITS.

Similarly, the new variable AWFCX(NX,NY) is the average product of field capacity and capillarity and DELTVX is the average reciprocal of field capacity multiplied by the time step DELTAT.

A modification has been also introduced to the initialization of the wetness parameter SWET. For most grid cells it assumes, as before, the value obtained in the run of the one-dimensional Gesima preprocessor. For the cells containing more then 80% of water surface SWET is changed be equal to that water coverage (a number between 0.8 and 1.0).

C.3 Subroutine INTNU

Since the uniform cloudiness has been replaced in the subroutine RADSFC (see Section C.7) by a two-dimensional variable SKYCO, the interpolation in space of its values from the large scale low resolution data has been included in INTNU.

Similarly, the interpolation in space of the mixing height XMIX, needed in the new version of MUGRAD (see Section C.5) has also been included. After interpolation from the large scale data, the Gesima terrain following height transformation is applied to XMIX.

The interpolation in time of SKYCO and XMIX is performed in subroutine TDBCNU.

C.4 Subroutine NUDEV

NUDEV is a new auxiliary subroutine, computing for output purposes the deviations of the mesoscale fields of wind, temperature and humidity computed by Gesima from their smooth, low resolution values interpolated from the large scale data and used in the "nudging" scheme.

The subroutine is called from the main program at INCOUT intervals. The three-dimensional deviation fields can be then written to output files in subroutine PRINTT. The vertical profiles of the minimum, maximum and mean deviations are written to the general output file (fort.06) in NUDEV.

C.5 Subroutine MUGRAD

MUGRAD is the main subroutine of the boundary layer module of Gesima. It has been modified, to include the new convective PBL parameterization, described in Section 4 of this report.

C.6 Subroutine PRINTT

This subroutine writes three-dimensional Gesima variables to the output files. For details see Section A1.9 of the last year report. The subroutine required extensions to accommodate the deviation arrays computed in subroutine NUDEV (see Section C.4). Instead of adding 4 more output files and increasing the size of the program, the deviation variables replaced in PRINTT some of the less needed output fields.

The temperature deviation is written out in place of the potential temperature to the unit IFOUTP(1). The deviations of u and v components replace the longwave radiation cooling and mass flux divergence in units IFOUTP(5) and IFOUTP(6), respectively. The humidity deviation from the large scale field replace the temperature deviation from the reference profile in IFOUTP(9).

C.7 Subroutine RADSFC

RADSFC computes the shortwave and longwave radiation fluxes at the ground surface. In the original Gesima two alternative approaches are used for parameterization of cloud effects on both solar and atmospheric radiation. For runs with the cloud module active, the "liquid water path", computed from the cloud liquid water content is used in RADSFC. If the cloud module is deactivated by setting the switch IFCLOU to 0 and the liquid water content is not available, Gesima uses the input cloud coverage parameter COV in a simplified set of radiation formulae.

Gesima is able to simulate only the stratiform clouds for the horizontal resolution of 20km, so the liquid water path approach was deactivated in Phase I of this project, and COV used instead, even in runs with cloud module active.

Extending the domain of Gesima made the use of a single input cloudiness parameter no longer reasonable. COV has been replaced in RADSFC by a two-dimensional array SKYCO, whose values are interpolated in time and space, from the large scale input data in subroutines INTNU and TDBCNU similarly to the meteorological fields used for "nudging" purposes.

C.8 Subroutine RLUSEX

Since the structure of the input land use data has changed, the subroutine RLUSE, reading and interpolating the land use information under the Phase I has been replaced by a new subroutine RLUSEX.

The interpolation of land use data is no longer necessary. RLUSEX reads the relative coverage of each grid cell by 8 classes of land use described in Section C.2 from eight input files: fort.31, fort.22, fort.23, fort.24, fort.35, fort.36, fort.37 and fort.38.

C.9 Subroutine RESTAR

Statements reading the new variables AWFCX, DELTVX and DIFCAP, computed in the subroutine INITS (see Section C.2) and written to the restart file in SAFETY, have been added to RESTAR.

C.10 Subroutine SAFETY

Statements writing to the restart file the new variables AWFCX, DELTVX and DIFCAP, computed in the subroutine INITS (see Section C.2), have been added to SAFETY.

C.11 Subroutine SURFW

The new variables DIFCAP, AWFCX and DELTVX, computed in subroutine INITS (see Section C.2) replaced reciprocals or products of XSOILS variables, where appropriate.

C.12 Subroutine TDBCNU

Statements interpolating in time the new variables XMIX and SKYCO have been added to TDBCNU.

C.13 Subroutine WRTAP

The purpose of this subroutine is to write the three-dimensional fields generated by Gesima to an unformatted output file, for later use by ADOM. The version used under Phase I wrote out more data than were actually needed, in order to enable the changes in the Gesima/ADOM interface without the need of rerunning Gesima. After gaining more experience, some of those

redundant fields have been removed in Phase II in order to save disc space.

C.14 Subroutine WRTAPF

After transferring the system from the Cray computer of the Ontario Centre of Large Scale Computations to the Centre Informatique de Dorval (CID), Gesima is run on the SX-3 supercomputer, while the Gesima/ADOM interface and ADOM use the CID Cray temporarily. This setup made the use of unformatted output file generated by WRTAP impossible.

Until ADOM is moved to SX-3, subroutine WRTAP must be replaced by its new, temporary version WRTAPF, using formatted write statements, instead of unformatted ones.

Since in the latest runs of Gesima the cloud module was disabled, the writing out of the cloud data have been removed from WRTAPF (and their use from the Gesima/ADOM interface). If the cloud module is reactivated, the removed statements in WRTAPF should be reactivated as well.

APPENDIX D

Gesima subroutines

APPENDIX D

Gesima Subroutines

This Appendix provides a list of all Gesima subroutines with short descriptions of their purposes and the meaning of formal parameters. For more information on subroutines developed or substantially modified under this project, see the Phase I report (Niewiadomski and Shenfeld, 1991). The modifications made in Phase II are described in detail in Appendix C of this report.

SUBROUTINE ADV(DC,C,ITYP)

Purpose: Compute advective terms of a central variable C and add them to the increment DC

Called from: ADVECN
Subroutines called: None
Origin: GKSS
Main modifications: None

Formal parameters:

DC(0:NXP1,0:NYP1,0:NZP1)	Increment array
C(0:NXP1,0:NYP1,0:NZP1)	Advected variable
ITYP	Switch depending of the type of adveced variable

SUBROUTINE ADVECN

Purpose: Call ADV for mass fluxes and temperature, perform auxiliary computations

Called from: MAIN
Subroutines called: ADV
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE BMUL(WL,WLS)

Purpose: Multiply B by WLS to obtain WL. Auxiliary subroutine of the pressure solver.

Called from: IGCG
Subroutines called: None
Origin: GKSS
Main modifications: None

Formal parameters: WL(NVOL), WLS(NVOL)

SUBROUTINE BORLAN(C)

Purpose: Apply Orlanski-type boundary conditions for variable C using phase velocity of temperature

Comments: This subroutine was used in the orginal model for temperature, humidity and hydrometeor mixing ratios. After introduction of subroutine BORLAQ is used only for temperature.

Called from: MAIN (if IFTINF.LE.0.OR.IFTOUT.LE.0)
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: C(0:NXP1,0:NYP1,0:NZP1)

SUBROUTINE BORLAQ(C)

Purpose: Apply Orlanski-type boundary conditions for variable C using phase velocity of humidity.

Comments: This is a modified subroutine BORLAN with phase velocities VPHT* replaced by VPHQ*. Applied for humidity and hydrometeor mixing ratios.

Called from: CLOUDP, HUMID (if IFQINF.LE.0.OR.IFQOUT.LE.0)

Subroutines called: None
Origin: MEP
Formal parameters: C(0:NXP1,0:NYP1,0:NZP1)

SUBROUTINE BOTTOM

Purpose: Compute u*, T* and q* if surface module is not called

Comments: Not used, since the surface module is always active in these simulations.

Called from: MAIN (if IFUBOT.EQ.3.AND.IFSURF.EQ.0)
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE CBOUND(C,IFI)

Purpose: Apply non-Orlanski lateral boundary conditions to variable C (temperature, humidity or hydrometeor mixing ratio)

Comments: IFI is equal to IFTINF for temperature or to IFQINF for other variables

Called from: MAIN, CLOUDP, HUMID
Subroutines called: None
Origin: GKSS

Main modifications: switch IFTINF is replaced by IFI which has been added as a formal parameter.

Formal parameters:
C(0:NXP1,0:NYP1,0:NZP1) the variable processed
IFI switch definig the type of boundary conditions

SUBROUTINE CENTUP

Purpose: Update the 'central variables' (wind components and temperature) by adding their increments

Comments: Humidity and hydrometeors are updated in HUMID and CLOUDP, respectively

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: Nudging terms added
Formal parameters: None

SUBROUTINE CLOUDP

Purpose: Compute transformations and transport of hydrometeors.

Comments: Driving subroutine of the cloud module. Not active in recent applications.

Called from: MAIN (if IFCLOU.EQ.1)

Subroutines called: TRANSP, DIFFC, TEMP, BORLAQ, CBOUND, QLIRTB
Origin: GKSS

Main modifications: Calls to BORLAN replaced by ones to BORLAQ
IFQINF included in CALL CBOUND statements.

Formal parameters: None

SUBROUTINE CONCMC(XCMC,YCMC,ALAT,ALON)

Purpose: Convert CMC coordinates to lat-lon

Comments: Based on the program CONVCMC received from OME. Used in older versions (which use RLUSE) only

Called from: RLUSE
Origin: MEP

Formal parameters:
XCMC, YCMC CMC coordinates (input)
ALAT, ALON latitude, longitude (output)

SUBROUTINE CONST

Purpose: Initialize various physical constants
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE CORIOL

Purpose: Compute the Coriolis force terms

Called from: MAIN (if IFCORI.GT.0)
Subroutines called: None
Origin: GKSS

Main modifications: Uniform geostrophic wind replaced by a 3-D array

Formal parameters: None

SUBROUTINE CUMU

Purpose: Compute the tendency terms for hydrometeors

Comments: This is the main subroutine of the cloud module. Not active in recent applications.

Called from: CLOUDP
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE DEFRAD

Purpose: Define some constants for the radiation module
Called from: MAIN (if IFRAD.EQ.1) at the beginning of each run

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE DIFFC(DC,C,M1T,M3T,ITYP)

Purpose: compute the diffusive source term for a centered variable C
Called from: CLOUDP, DIFFIL, HUMID (if IFDIFF.NE.0)

Subroutines called: IMPDI2
Origin: GKSS
Main modifications: None

Formal parameters:

C(0:NXP1,0:NYP1,0:NZP1)	variable processed
DC(0:NXP1,0:NYP1,0:NZP1)	increment array
M1T(0:NXP1,0:NYP1,0:NZP1)	horizontal diffusivity
M3T(0:NXP1,0:NYP1,0:NZP1)	vertical diffusivity
ITYP	passed to IMPDI2

SUBROUTINE DIFFIL

Purpose: Call DIFFC and FILTER for wind and temperature. Convert temperature to real value before that and back to deviation form after.
Called from: MAIN (if IFDIFF.NE.0.OR.IFFILT.NE.0)

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE DISPLU

Purpose: Compute velocities from fluxes

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE FBOUND

Purpose: Compute non-Orlanski boundary terms for wind

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE FGRAD(C)

Purpose: Compute pressure gradient and update fluxes to conserve mass.

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None

Formal parameters:
C(0:NXP1,0:NYP1,0:NZP1) variable processed. Actually XPRES only.

SUBROUTINE FILTER(DC1D,C)

Purpose: Apply 3 or 5-point filter to variable C
Called from: DIFFIL, HUMID (if IFFILT.NE.0)

Subroutines called: None
Origin: GKSS

Main modifications: None
Formal parameters: None

SUBROUTINE FLUCOR

Purpose: Compute new inflow rate, check balance and adjust outflow.

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE FLUXFI

Purpose: Find final fluxes by taking the mean of old and corrector values

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE FLUXUP

Purpose: Compute fluxes from velocities

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE FORLAN

Purpose: Apply Orlanski boundary conditions to fluxes

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE HUMID

Purpose: Solve the humidity equation.
Called from: MAIN (if IFHUMI.EQ.1)

Subroutines called: TRANSP, DIFFC, FILTER, BORLAQ, CBOUND, QVTOB

Origin: GKSS

Main modifications: Call to BORLAN replaced by one to BORLAQ.
IFQINF added as formal parameter of CBOUND.
Nudging terms added

Formal parameters: None

SUBROUTINE HYHORI

Purpose: Compute horizontal hydrostatic pressure gradient
Called from: MAIN (if IFHYGR.EQ.1)

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE HYVERT

Purpose: Compute vertical hydrostatic pressure gradient
Called from: MAIN (if IFHYGR.EQ.1 and IFSEMI.NE.0)

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE IBOUND

Purpose: Initialize some surface parameters if IFSURF = 0

Comments: Not used in this application, since the surface module is always active (IFSURF = 1)

Called from: MAIN (if IFSURF.EQ.0 and IFHOTS.EQ.0)

Subroutines called: None
Origin: GKSS

Main modifications: None
Formal parameters: None

SUBROUTINE IGCG

Purpose: Solves a linear system of equations by preconditioned conjugate gradient method

Comments: Main subroutine of the pressure solver

Called from: MAIN
Subroutines called: BMUL, LIMUL, UIMUL
Origin: GKSS
Main modifications: Some informative output removed
Formal parameters: None

SUBROUTINE IJKPOS(INDEX,I,J,K)

Purpose: Calculate indices (i,j,k) from 1-D index of a centered variable
Comments: Auxiliary subroutine, not used in this version

Called from: not used in this version
Subroutines called: None
Origin: GKSS
Main modifications: None

Formal parameterers:
INDEX index of a 1-D array (input)
I,J,K indices of the equivalent 3-D array (output)

SUBROUTINE IMBOUY

Purpose: Computes buoyancy terms

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE IMPDI2(DC1D,C1D,IM3T2D,ITYP)

Purpose: Compute implicit vertical diffusion

Called from: DIFFC
Subroutines called: LUSOL2
Origin: GKSS

Main modifications: Not used part for ITYP=4 removed

Formal parameters:
C1D(NVOL) variable processed
DC1D(NVOL) incerment array
IM3T2D(NH2,0:NZP1) diffusivity array
ITYP Type of variable processed:
ITYP = 1 for temperature, moisture, hydrometeors
ITYP = 2 for horizontal velocities
ITYP = 3 for vertical velocity
ITYP = 4 for passive tracer

SUBROUTINE INIFLA

Purpose: Initialize fluxes according to initial velocity fields
Comments: based on subroutine FLUXUP
replaces subroutine INITFL
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: None
Origin: MEP
Formal parameters: None

SUBROUTINE INITCL

Purpose: Initialize hydrometeor fields and some contstants of the cloud module

Comments: Hydrometeors set to 0 for initial runs only

Called from: MAIN at the beginning of each run

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE INITFL

Purpose: Initialize inflow flux profiles

Comments: Not used in this version, replaced by INIFLA
Called from: Not used in this version, replaced by INIFLA

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE INITFT

Purpose: Adjust boundaries for flux-conservation and compute total flux
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE INITNU

Purpose: Initialize interpolation coefficients for nudging and boundary conditions.
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called:	None
Origin:	MEP
Formal parameters:	None

SUBROUTINE INITS

Purpose: Initialize surface model constants and variables
Called from: MAIN (if IFSURF.EQ.1) at the beginning of each run

Subroutines called:	None
Origin:	GKSS
Main modifications:	SOILS redefined, XSOIL introduced. DIFCAP, AWFCX, DELTVX variables introduced in Phase II, see Appendix C)
Formal parameters:	None

SUBROUTINE INITUR

Purpose: Initialize constants of the turbulence module
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called:	KBOUND
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE INTBC

Purpose: Interpolate time dependent boundary conditions

Comments: Mostly obsolete, since for most variables t.d.b.c. have been replaced by nudging.

Called from: MAIN at the beginning of each run and every full hour

Subroutines called: None
Origin: MEP
Formal parameters: None

SUBROUTINE INTINI

Purpose: Initialize interpolation coefficients for boundary conditions

Comments: Used in pre-August 1991 versions only

Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: None
Origin: MEP
Formal parameters: None

SUBROUTINE INTNU

Purpose: Interpolate nudging fields, sky coverage and mixed layer height.

Comments: Modified in Phase II, see Appendix C.

Called from: RDBCI at the beginning of an initial run and MAIN at the beginning of a restart run and every full hour

Subroutines called: None
Origin: MEP
Formal parameters: None

SUBROUTINE INZRTP

Purpose: Initialize reference density, Orlanski phase velocities and some other variables.
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: None
Origin: GKSS

Main modifications: Phase velocities for humidity type variables (VPHQE etc.) added.

Formal parameters: None

SUBROUTINE KBOUND

Purpose: Apply boundary conditions for turbulent diffusion coefficients

Comments: Active only if IFDIFF.GE.2

Called from: INITUR, MUGRAD
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE LIMUL(WLS,WL)

Purpose: Multiply the inverse of L with WL to obtain WLS

Called from: IGCG
Subroutines called: None
Origin: GKSS
Main modifications: None

Formal parameters:
WL(NVOL) operand array
WLS(NVOL) product array

SUBROUTINE LUSOL2(A,B,C,F,X,N,NH2)

Purpose: solve a tridiagonal matrix using Thomas algorithm

Called from: IMPDI2, SURFW
Subroutines called: None
Origin: GKSS
Main modifications: None

Formal parameters:
A(NH2,0:N),B(NH2,0:N),C(NH2,0:N),F(NH2,0:N) coefficient arrays
X(NH2,0:N) processed array
N,NH2 array dimensions

SUBROUTINE LWRAD

Purpose: Compute longwave radiation fluxes and flux divergence

Comments: Not used in this application (IFRAD set to 0)

Called from:	MAIN (if IFRAD.EQ.1)
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE MOMFLU

Purpose: Compute momentum flux for output purposes

Called from:	MAIN at INCOUT intervals
Subroutines called:	None
Origin:	GKSS
Main modifications:	3-D geostrophic wind introduced
Formal parameters:	None

SUBROUTINE MOMFNO

Purpose: Compute analytic hydrostatic momentum flux for scaling

Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE MONITO

Purpose: Compute and print max and min values of some parameters

Comments: Used to monitor propper behaviour of the model

Called from:	MAIN at IFMONI intervals
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE MUGRAD

Purpose: Compute eddy diffusivity coefficients

Comments: New convective PBL parameterization introduced

Called from:	MAIN (if IFDIFF.EQ.2)
Subroutines called:	STRATI, KBOUND
Origin:	GKSS
Main modifications:	See Appendix C
Formal parameters:	None

SUBROUTINE NEWOLD

Purpose: Replace 'old' velocities and temperature with the 'new' ones.

Called from: MAIN at the end of each time step

Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE NUDEV

Purpose: Compute deviations from the nudging fields for output purposes.
Compute and print max, min and average values of velocity, temperature and humidity

Comments: Developed in Phase II, see Appendix C.

Called from:	MAIN at INCOUT intervals
Subroutines called:	None
Origin:	MEP
Formal parameters:	None

SUBROUTINE NUDGING

Purpose: Compute the nudging terms

Called from:	MAIN
Subroutines called:	None
Origin:	MEP
Formal parameters:	None

SUBROUTINE ORLAN

Purpose: Set phase velocities equal to outflow velocities and determine the Courant number

Called from: MAIN
Subroutines called: None
Origin: GKSS

Main modifications: Separate (from temperature) phase velocities for humidity and hydrometeors introduced
Formal parameters: None

SUBROUTINE OUTERF

Purpose: Adjust outer values for all fluxes

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE PHYDRO(C1D)

Purpose: Compute the hydrostatic pressure field

Called from: MAIN (if IFHYUP.EQ.1)
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters:
C1D(NVOL) Temperature deviation array

SUBROUTINE PLHS

Purpose: Compute the left hand side of the Poisson equation for pressure
Comments: Part of the pressure solver package
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE PRECG

Purpose:	Compute the right hand side of the Poisson equation for pressure
Comments:	Part of the pressure solver package

Called from:	MAIN
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE PRIGEO

Purpose:	Print geometry of grid
Comments:	Auxiliary subroutine, not used in this version

Called from:	not used in this version
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE PRINTT

Purpose:	Write 3-D arrays of specified parameters to output files
Comments:	Main output subroutine of the model

Called from:	MAIN
Subroutines called:	None
Origin:	GKSS
Main modifications:	Some formats changed. Some fieds redefined in Phase II, see Appendix C.
Formal parameters:	None

SUBROUTINE QLIRTB

Purpose:	Assign top and bottom boundary conditions for hydrometeors

Called from:	CLOUDP
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE QVTOB

Purpose: Assign top and bottom boundary conditions for humidity

Called from: HUMID
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE RADSFC

Purpose: Compute surface radiation fluxes

Comments: For IFRAD=0 (as is the case for this application) this subroutine parameterizes the longwave radiation, which for IFRAD=1 is computed in LWRAD

Modified in Phase II, see Appendix C.

Called from: MAIN (if IFSURF.EQ.1)
Subroutines called: None
Origin: GKSS
Main modifications: See Appendix C.
Formal parameters: None

SUBROUTINE RDBCI

Purpose: Read boundary conditions and nudging data. Initialize some variables.

Comments: A version of RDBC for the initial runs.
Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: INTNU
Origin: MEP
Formal parameters: None

SUBROUTINE RDBC

Purpose: Read boundary conditions and nudging data.

Called from: MAIN at the beginning of a restart run and every full hour

Subroutines called: None
Origin: MEP
Formal parameters: None

SUBROUTINE RDTAPE

Purpose: Read initial profiles from the output of 1-D run

Comments: Most parameters overwritten in RDBCI

Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: None
Origin: GKSS

Main modifications: Structure of 1-D output and the read statements slightly changed.
Formal parameters: None

SUBROUTINE READD

Purpose: Read the input file and initialize some constants

Comments: For the detailed structure of the input file see Appendix B

Called from: MAIN at the beginning of each run

Subroutines called: None
Origin: GKSS
Main modifications: Some namelists redefined.
Reading topography data moved to RDPROF (for IFTOPO = 0 only).
Grid data read in from input redefined inside the subroutine.

Formal parameters: None

SUBROUTINE RLUSE

Purpose: Read and interpolate land use data.
Comments: Used in older versions of the model. If the interpolated land use data are available, RLUSEX is called instead.

Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called: CONCMC
Origin: MEP
Formal parameters: None

SUBROUTINE RLUSEX

Purpose: Read land use data.

Comments: Developed in Phase II to replace RLUSE if the interpolated land use data are available. Each category is read from a different file.The subroutine is domain-dependent. For details see Appendix C.

Called from: MAIN (if IFHOTS.EQ.0 - initial run only)

Subroutines called:	None
Origin:	MEP
Formal parameters:	None

SUBROUTINE RESTAR

Purpose: Read the unformatted restart file

Called from: MAIN (if IFHOTS.EQ.1 - at the beginning of a restart run)

Subroutines called:	None
Origin:	GKSS
Main modifications:	See Appendix C
Formal parameters:	None

SUBROUTINE RTOPO

Purpose: Read topography data

Called from: MAIN (if IFTOPO.EQ.0 and IFHOTS.EQ.0) at the beginning of an initial run only.

Subroutines called:	None
Origin:	MEP
Formal parameters:	None

SUBROUTINE SAFETY(NTAPE)

Purpose: Write an unformatted restart file

Comments: A single NTAPE value and single calls to SAFETY used in this version, instead of the double calls in original Gesima.

Called from:	MAIN at INCHOT intervals
Subroutines called:	None

Origin: GKSS
Main modifications: See Appendix C
Formal parameters: None

SUBROUTINE SETIND

Purpose: Set indicator arrays for inflow/outflow

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE SHIFTT

Purpose: Define shift coefficients
Compute velocities from fluxes at the beginning of a corrector step.

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE SPRINT

Purpose: Write some surface module parameters to an output file

Called from: MAIN at incout intervals (if IFSURF.EQ.1)

Subroutines called: None
Origin: GKSS
Main modifications: Some parts removed
Formal parameters: None

SUBROUTINE STAU

Purpose: Compute auxiliary variable TAU1D

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None

Formal parameters: None

SUBROUTINE STRATI

Purpose: Compute auxiliary terms for diffusivity parameterization

Called from: MUGRAD
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE SURFW

Purpose: Compute the surface energy balance
Comments: Main subroutine of the surface module

Called from: MAIN (if IFSURF.EQ.1)
Subroutines called: LUSOL2
Origin: GKSS

Main modifications: SOILS replaced by XSOIL. DIFCAP, AWFCX and DELTVX introduced, see Appendix C.

Formal parameters: None

SUBROUTINE TDBCNU

Purpose: Assume new values of nudging variables, cloudiness and mixed layer height.
Assume new inflow boundary conditions.

Comments: The scheme defining the boundary conditions for hydrometeors not tested sufficiently (but the cloud module not active in recent simulations). Interpolation of cloudiness and mixing height introduced in Phase II.

Called from: MAIN
Subroutines called: None
Origin: MEP
Formal parameters: None

SUBROUTINE TEMP

Purpose: Convert temperature deviation TNC to actual absolute temperature.

Comments: Used mainly for output purposes

Called from:	MAIN
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE TIMSTP

Purpose: Compute DELTAT from numerical stability criteria for runs with variable time step

Comments: Not tested and not used in this application, (IFTIM set to 0 - constant time steps)

Called from:	MAIN (if IFTIM.EQ.1)
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None

SUBROUTINE TRANSP(DC1D,C1D,W)

Purpose: Compute advective transport of passive components using Smolarkiewicz scheme

Called from:	CLOUDP, HUMID
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	
C1D(NVOL)	processed variable
DC1D(NVOL)	increment array
W(0:NXP1,0:NYP1,0:NZP1)	sedimentation velocity

SUBROUTINE TTOP

Purpose: Top boundary conditions for temperature

Called from:	MAIN
Subroutines called:	None
Origin:	GKSS

Main modifications: None
Formal parameters: None

SUBROUTINE UIMUL(WLS,WL)

Purpose: Multiply the inverse of U by WL to obtain WLS
Comments: Part of the pressure solver package

Called from: IGCG
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters:
WL(NVOL) operand array
WLS(NVOL) product array

SUBROUTINE UVTBOT

Purpose: Lower boundary conditions for U, V , W, T

Called from: MAIN
Subroutines called: None
Origin: GKSS
Main modifications: None
Formal parameters: None

SUBROUTINE VERIFY

Purpose: Print some input/restart parameters
Comments: Auxiliary subroutine
Called from: MAIN at the beginning of each run

Subroutines called: None
Origin: GKSS
Main modifications: Some output removed
Formal parameters: None

SUBROUTINE WRTAP(NTAPE)

Purpose: Write binary output data for ADOM purposes

Comments: Based on subroutine SAFETY.
Some fields removed in Phase II - see Appendix C.
Temporarily replaced by WRTAPFX - see Appendix C.

Called from: MAIN at INTAP intervals
Subroutines called: None
Origin: MEP
Formal parameters: None

SUBROUTINE WRTAPF(NTAPE)

Purpose: Write formatted output data for ADOM purposes

Comments: Temporary replacement of subroutine WRTAP, see Appendix C.

Called from:	MAIN at INTAP intervals
Subroutines called:	None
Origin:	MEP
Formal parameters:	None

SUBROUTINE WTOPBO

Purpose: Update top and bottom b. c. for vertical flux

Called from:	MAIN
Subroutines called:	None
Origin:	GKSS
Main modifications:	None
Formal parameters:	None